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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:53:55 ON 31 JAN 2007

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

1.05

1.05

FILE 'REGISTRY' ENTERED AT 10:57:03 ON 31 JAN 2007

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STRUCTURE FILE UPDATES: 30 JAN 2007 HIGHEST RN 918865-48-2

DICTIONARY FILE UPDATES: 30 JAN 2007 HIGHEST RN 918865-48-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

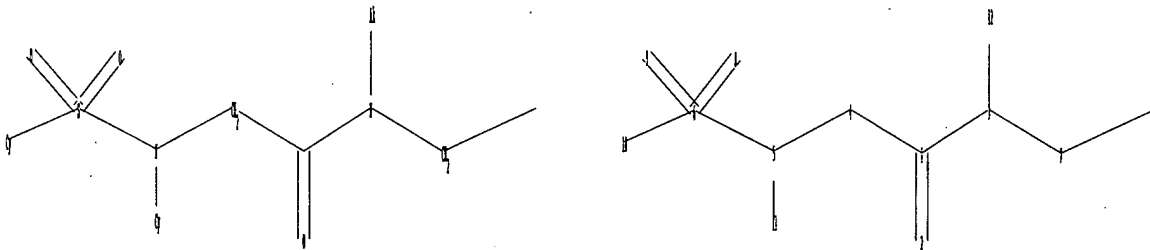
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10529637-exam-broad.str



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 14

chain bonds :

1-2 1-3 1-4 3-7 3-12 4-5 5-6 5-11 6-8 6-9 6-10 7-14

exact/norm bonds :

1-2 1-3 1-4 3-7 3-12 4-5 5-6 5-11 6-8 6-9 6-10 7-14

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

10:Atom 11:Atom 12:CLASS 14:CLASS

Generic attributes :

12:

Saturation : Saturated

STN STRUCTURE SEARCH.

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptayvv1621

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS	4	OCT 30	CHEMLIST enhanced with new search and display field
NEWS	5	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS	6	NOV 10	CA/Caplus F-Term thesaurus enhanced
NEWS	7	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS	8	NOV 20	CA/Caplus to MARPAT accession number crossover limit increased to 50,000
NEWS	9	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS	10	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS	11	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS	12	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS	13	DEC 18	CA/Caplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS	14	DEC 18	CA/Caplus patent kind codes updated
NEWS	15	DEC 18	MARPAT to CA/Caplus accession number crossover limit increased to 50,000
NEWS	16	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS	17	DEC 27	CA/Caplus enhanced with more pre-1907 records
NEWS	18	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS	19	JAN 16	CA/Caplus Company Name Thesaurus enhanced and reloaded
NEWS	20	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS	21	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS	22	JAN 22	CA/Caplus updated with revised CAS roles
NEWS	23	JAN 22	CA/Caplus enhanced with patent applications from India
NEWS	24	JAN 29	PHAR reloaded with new search and display fields
NEWS	25	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS EXPRESS	NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.		
NEWS HOURS	STN Operating Hours Plus Help Desk Availability		
NEWS LOGIN	Welcome Banner and News Items		
NEWS IPC8	For general information regarding STN implementation of IPC 8		
NEWS X25	X.25 communication option no longer available		

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Number of Carbon Atoms : less than 7

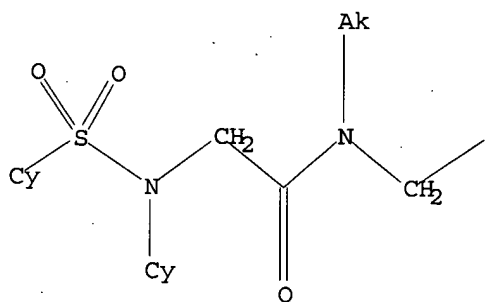
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Node 12: Limited
C,C1-6

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 10:57:37 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2068 TO ITERATE

96.7% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

28 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 38633 TO 44087
PROJECTED ANSWERS: 257 TO 901

L2 28 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 10:57:43 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 40272 TO ITERATE

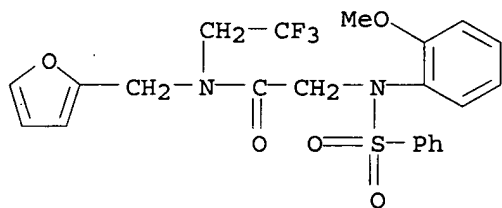
100.0% PROCESSED 40272 ITERATIONS
SEARCH TIME: 00.00.01

507 ANSWERS

L3 507 SEA SSS FUL L1

=> d l3 scan

L3 507 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C22 H21 F3 N2 O5 S



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

172.55

173.60

FILE 'CAPLUS' ENTERED AT 10:58:27 ON 31 JAN 2007

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FILE COVERS 1907 - 31 Jan 2007 VOL 146 ISS 6

FILE LAST UPDATED: 30 Jan 2007 (20070130/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 13

L4 16 L3

=> s 14 not py > 2004

2662812 PY > 2004

L5 11 L4 NOT PY > 2004

=> s 15 not 529637

0 529637

L6 11 L5 NOT 529637

=> d 16 abs ibib hitstr 1-

YOU HAVE REQUESTED DATA FROM 11 ANSWERS - CONTINUE? Y/(N):y

L6 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

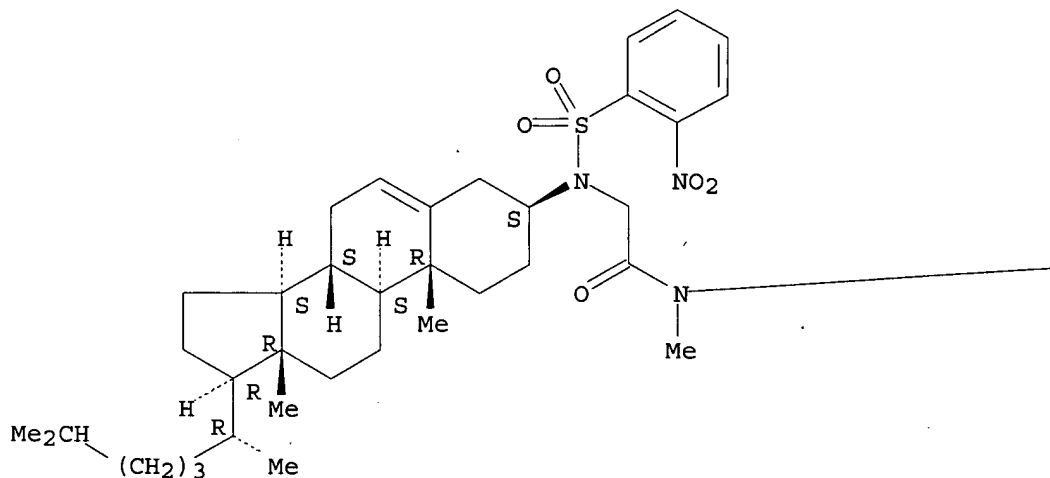
AB The authors report the synthesis of 7 α -substituted β -estradiol derivs. bearing side chains terminated with cholesterol and 3 β -cholesterylamine. These chimeric compds. were designed to exhibit

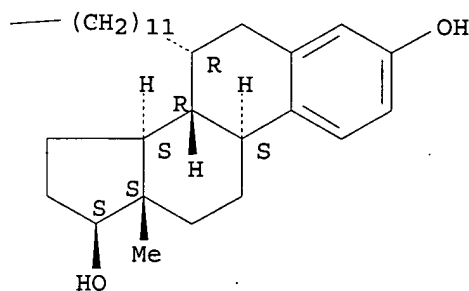
high affinity for estrogen receptors (ERs) and cellular plasma membranes to potentially enable regulated uptake of ERs by mammalian cells. Evaluation with recombinant yeast reporting compound-mediated ER dimerization revealed potencies similar to the antiestrogen ICI 182780. Compds. that efficiently deliver dominant neg. ERs into cells may provide novel therapeutics against breast cancers.

ACCESSION NUMBER: 2002:14237 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 136:216932
TITLE: Synthesis of Chimeric 7 α -Substituted Estradiol Derivatives Linked to Cholesterol and Cholesterylamine
AUTHOR(S): Hussey, Stephen L.; He, Enfei; Peterson, Blake R.
CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Organic Letters (2002), 4(3), 415-418
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:216932
IT 402570-31-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and estrogen receptor affinity of estradiol-cholesterol and -cholesterylamine derivs. as potential anticancer agents)
RN 402570-31-4 CAPLUS
CN Acetamide, 2-[(3 β)-cholest-5-en-3-yl] [(2-nitrophenyl)sulfonyl]amino]-N-[11-[(7 α ,17 β)-3,17-dihydroxyestra-1,3,5(10)-trien-7-yl]undecyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 AB X1X2X3CC(R1)(ArYR2)CX4X5X6 (Ar = aryl; R1 = OH, CO2H, alkoxy, alkylcarbonyloxy, heteroalkyloxy, etc.; R2 = alkyl, heteroalkyl, aryl, aralkyl; X1-X6 = H, alkyl, heteroalkyl, F, Cl; Y = NR12SOm, NR12CO, NR12CONR13, NR12CO2, etc.; m = 1, 2; R12, R13 = H, alkyl, heteroalkyl, aryl, aralkyl, etc.; with provisos), were prepared Thus, 4-(hexafluoro-2-hydroxyisopropyl)aniline in MeOH was treated with PhSO2Cl to give 4-[HO(CF3)2C]C6H4NHSO2Ph. The latter showed LXR α with EC50 <2 μ M.

ACCESSION NUMBER: 2000:666587 CAPLUS <<LOGINID::20070131>>
 DOCUMENT NUMBER: 133:237693
 TITLE: Preparation of bis(trifluoromethyl)hydroxymethylbenzenesulfonamides, -ureas, and -carbamates as liver X receptor modulators.
 INVENTOR(S): Li, Leping; Medina, Julio C.; Hasegawa, Hirohiko; Cutler, Serena T.; Liu, Jiwen; Zhu, Liusheng; Shan, Bei; Lustig, Kevin
 PATENT ASSIGNEE(S): Tularik Inc., USA
 SOURCE: PCT Int. Appl., 113 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000054759	A2	20000921	WO 2000-US6611	20000315
WO 2000054759	A3	20010215		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,				

CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6316503	B1	20011113	US 2000-525861	20000314
CA 2367595	A1	20000921	CA 2000-2367595	20000315
EP 1161233	A2	20011212	EP 2000-914958	20000315

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO

JP 2002539155	T	20021119	JP 2000-604835	20000315
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PRIORITY APPLN. INFO.: US 1999-124525P P 19990315
WO 2000-US6611 W 20000315

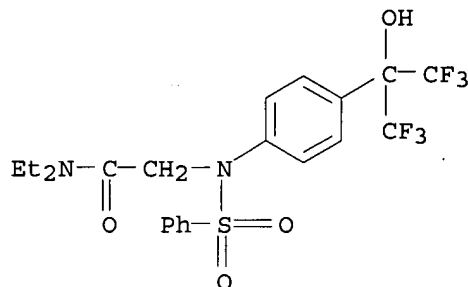
OTHER SOURCE(S): MARPAT 133:237693

IT 293754-48-0P

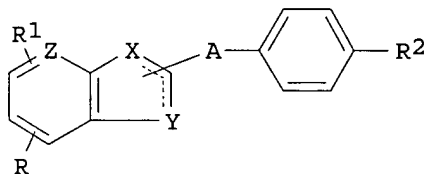
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bis(trifluoromethyl)hydroxymethylbenzenesulfonamides, -ureas, and -carbamates as liver X receptor modulators)

RN 293754-48-0 CAPLUS

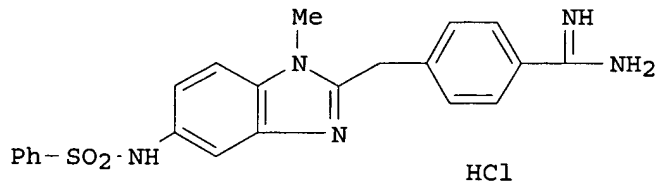
CN Acetamide, N,N-diethyl-2-[(phenylsulfonyl)[4-[2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl]amino]- (9CI) (CA INDEX NAME)



L6 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
GI



I



HCl

II

AB Title compds. [I; R = 5-C6H5SO2NH, 6-C6H5SO2NH, 5-C6H5NHSO2,
5-C6H5SO2N(CH2COOEt), 5-C6H5SO2N(CH3), 5-C6H5N(CH2CH2CH2COOEt)CO, 5-C6H5,

CH3N(C6H5)CO, 8; R1 = H, 7-CH3, 3-Br, 3-EtO; R2 = C(:NH)NH2; A = CH2, NH; X = CH, MeN, EtOCOCH2CH2N, O, S, NCH2CO2H; Y = N, CH, CH:CH; Z = CH, N; dotted bond = single, double in relation to X; A is attached at 2, or 8 position depending on the heterocyclic ring] and their tautomers, stereoisomers, mixts. and their physiol. compatible salts with inorg. or organic acids or bases are prepared and title compds in which R2 is a cyano group, present valuable intermediate products for the production of the remaining compds. of the general formula I, with R2 is amidino, which have valuable pharmacol. properties, especially an antithrombotic activity. Thus, the title compound II was prepared

ACCESSION NUMBER: 1999:511140 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 131:157771
TITLE: Preparation of five-membered, benzo-condensed heterocycles as antithrombotics
INVENTOR(S): Ries, Uwe; Haeu, Norbert; Mihm, Gerhard; Priepeke, Henning; Binder, Klaus; Stassen, Jean Marie; Wienen, Wolfgang; Zimmermann, Rainer
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma Kg, Germany
SOURCE: PCT Int. Appl., 250 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9940072	A1	19990812	WO 1999-EP537	19990128
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19804085	A1	19990805	DE 1998-19804085	19980203
DE 19834325	A1	20000217	DE 1998-19834325	19980730
CA 2319494	A1	19990812	CA 1999-2319494	19990128
AU 9927201	A	19990823	AU 1999-27201	19990128
EP 1060166	A1	20001220	EP 1999-907437	19990128
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002502844	T	20020129	JP 2000-530502	19990128
PRIORITY APPLN. INFO.:			DE 1998-19804085	A 19980203
			DE 1998-19834325	A 19980730
			WO 1999-EP537	W 19990128

OTHER SOURCE(S): MARPAT 131:157771

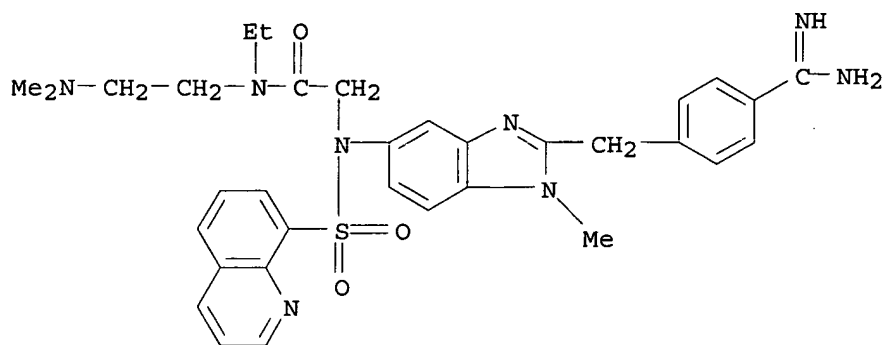
IT 236415-28-4P 236415-95-5P 236415-97-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of five-membered benzo-condensed heterocycles as antithrombotics)

RN 236415-28-4 CAPLUS

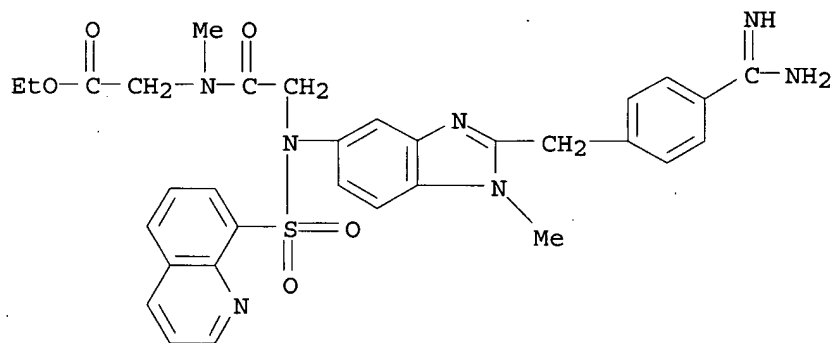
CN Acetamide, 2-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl](8-quinolinylsulfonyl)amino]-N-[2-(dimethylamino)ethyl]-N-ethyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

RN 236415-95-5 CAPLUS

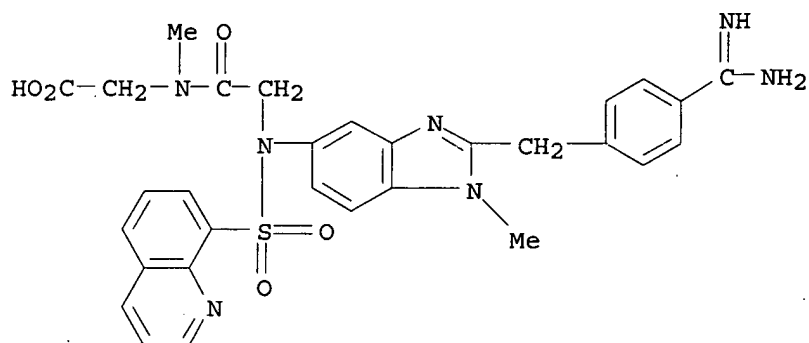
CN Glycine, N-[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 236415-97-7 CAPLUS

CN Glycine, N-[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 AB Approx. 300 antithrombotic title compds. such as 4-[5-[N-(8-quinolylsulfonyl)-N-(carboxymethyl)amino]-1-methyl-1H-benzimidazol-2-ylmethyl]benzamidinium hydrochloride (I), 4-[5-[N-(benzenesulfonyl)-N-[2-(dimethylamino)ethyl]amino]-1-benzyl-1H-benzimidazol-2-ylmethyl]benzamidinium dihydrochloride, 4-[5-[N-(3-carboxypropionyl)-N-(cyclopentyl)amino]-1-methyl-1H-benzimidazol-2-ylmethyl]benzamidinium hydrochloride (II), and 4-[5-[N-(8-quinolylsulfonyl)-N-(carboxymethyl)amino]-1-methyl-1H-benzothiazol-2-ylmethyl]benzamidinium hydrochloride were prepared by standard methods. The ED200 in μM for I was 0.92 and for II was 0.82. Formulations for the antithrombotics were given.

ACCESSION NUMBER: 1999:505930 CAPLUS <<LOGINID::20070131>>
 DOCUMENT NUMBER: 131:157761
 TITLE: 5-Membered heterocyclic condensed benzo derivatives, their preparation, and their use as drugs
 INVENTOR(S): Ries, Uwe; Haeu, Norbert; Mihm, Gerhard; Priepke, Henning; Binder, Klaus; Stassen, Jean Marie; Wienen, Wolfgang; Zimmermann, Rainer
 PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
 SOURCE: Ger. Offen., 94 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19804085	A1	19990805	DE 1998-19804085	19980203
CA 2319494	A1	19990812	CA 1999-2319494	19990128
WO 9940072	A1	19990812	WO 1999-EP537	19990128
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9927201	A	19990823	AU 1999-27201	19990128

EP 1060166	A1	20001220	EP 1999-907437	19990128
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002502844	T	20020129	JP 2000-530502	19990128
US 6114532	A	20000905	US 1999-243200	19990202

PRIORITY APPLN. INFO.:

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WO 1999-EP537	W	19990128

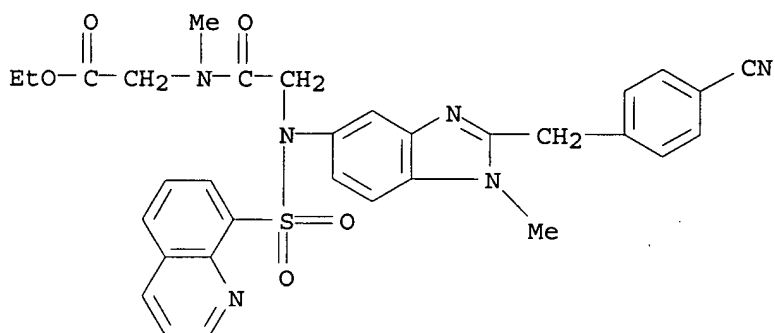
OTHER SOURCE(S): MARPAT 131:157761

IT 237751-41-6 237752-24-8

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and antithrombotic activity of benzimidazolylmethylbenzamidines)

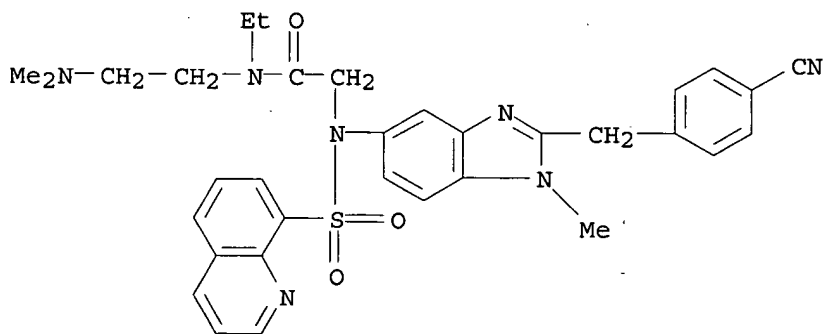
RN 237751-41-6 CAPLUS

CN Glycine, N-[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 237752-24-8 CAPLUS

CN Acetamide, 2-[[2-[(4-cyanophenyl)methyl]-1-methyl-1H-benzimidazol-5-yl](8-quinolinylsulfonyl)amino]-N-[2-(dimethylamino)ethyl]-N-ethyl- (9CI) (CA INDEX NAME)

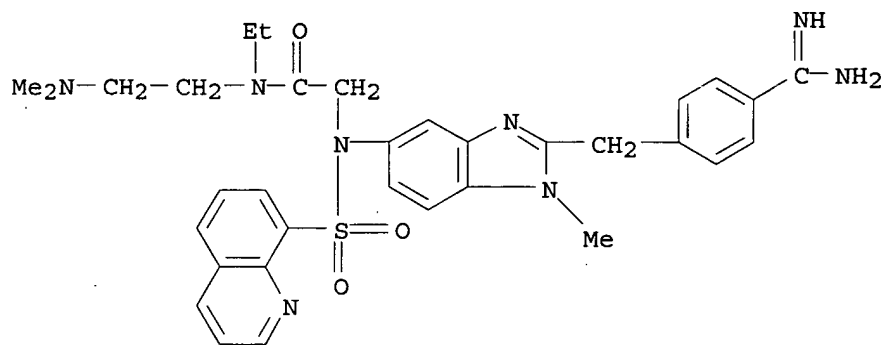


IT 236415-28-4P 236415-95-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antithrombotic activity of benzimidazolylmethylbenzamidines)

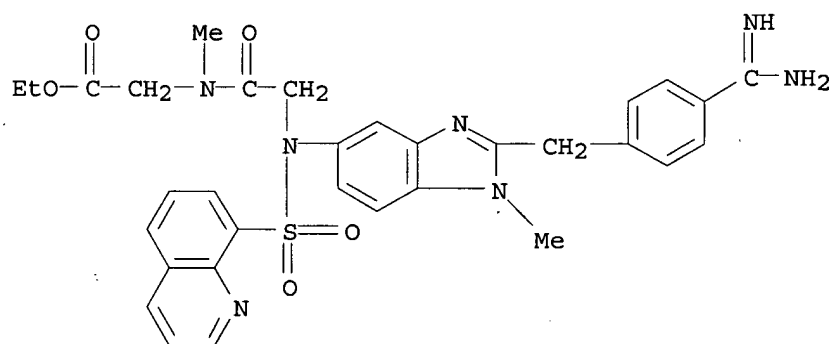
RN 236415-28-4 CAPLUS

CN Acetamide, 2-[[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl](8-quinolinylsulfonyl)amino]-N-[2-(dimethylamino)ethyl]-N-ethyl-, dihydrochloride (9CI) (CA INDEX NAME)



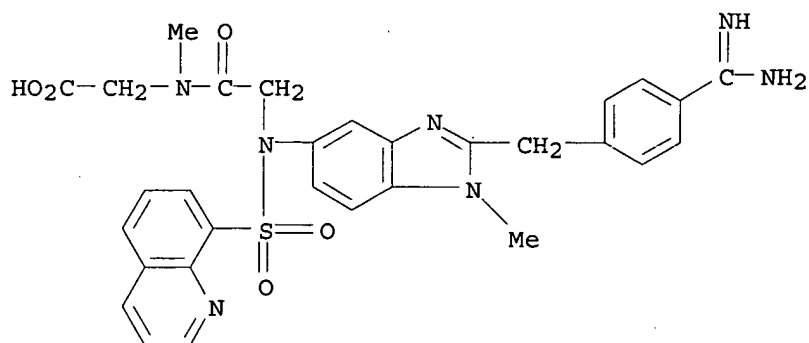
● 2 HCl

RN 236415-95-5 CAPLUS
 CN Glycine, N-[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



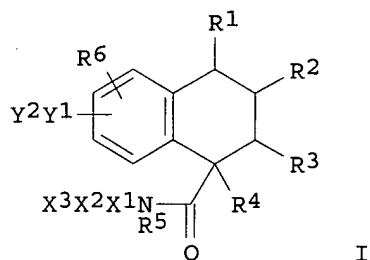
● HCl

IT 236415-97-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and antithrombotic activity of benzimidazolylmethylbenzamidines)
 RN 236415-97-7 CAPLUS
 CN Glycine, N-[2-[[4-(aminoiminomethyl)phenyl]methyl]-1-methyl-1H-benzimidazol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L6 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
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AB Title compds. [I; R1-R4 = H, or R1, R2 = H, R3R4 = double bond, or R1R2 and R3R4 = double bonds; R5 = H, alkyl; R6 = H, F, Cl, Br, alkyl; X1 = alkylene; X2 = phenylene, cycloalkylene, thienylene, oxazolylylene, thiazolylylene, imidazolylylene, pyridinylylene, pyrimidinylylene, pyrazinylylene, pyridazinylylene; X3 = cyano, amino, 2-amino-1H-imidazol-4-yl, etc.; Y1 = O, RbN, RbNSO2, RbNCO, etc.; Rb = H, (substituted) alkyl, phenylalkyl, naphthylalkyl, aminocarbonyl, etc.; Y2 = alkyl, cycloalkyl, (substituted) aminocarbonylalkyl, Ph, naphthyl, pyrrolyl, thiazolyl, thienyl, pyridinyl, etc.], were prepared Thus, Et [2-[quinolin-8-sulfonyl-[5-(carbamidoylbenzylcarbamoyl)-3,4-dihydronaphthalen-2-yl]amino]acetyl]amino]acetate hydrochloride showed a thrombin time ED200 = 0.009 μ M.

ACCESSION NUMBER:	1999:384101 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER:	131:44664
TITLE:	Preparation of carbamoylnaphthalenes as thrombin inhibitors.
INVENTOR(S):	Soyka, Rainer; Heckel, Armin; Lehmann-Lintz, Thorsten; Walter, Rainer; Wienen, Wolfgang; Stassen, Jean Marie
PATENT ASSIGNEE(S):	Boehringer Ingelheim Pharma K.-G., Germany
SOURCE:	Ger. Offen., 92 pp.
	CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19754490	A1	19990610	DE 1997-19754490	19971209
WO 9929670	A2	19990617	WO 1998-EP7958	19981208
WO 9929670	A3	19990910		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9918773	A	19990628	AU 1999-18773	19981208
PRIORITY APPLN. INFO.:			DE 1997-19754490	A 19971209
			WO 1998-EP7958	W 19981208

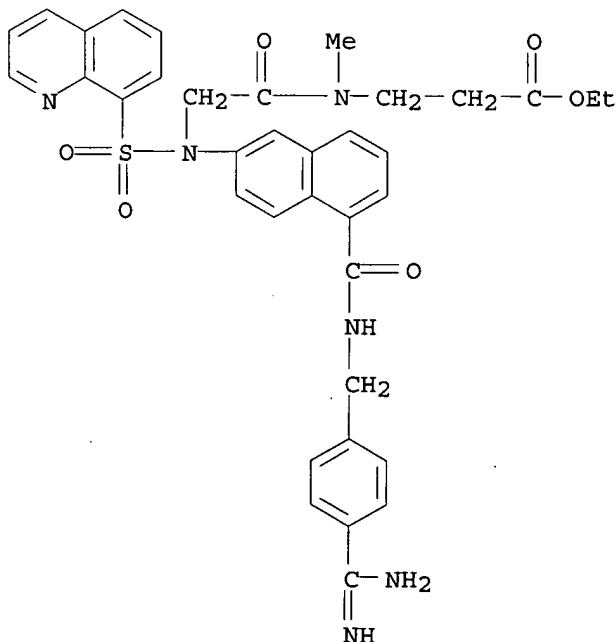
OTHER SOURCE(S): MARPAT 131:44664

IT 227276-66-6P 227276-68-8P 227276-69-9P
227276-71-3P 227276-76-8P 227276-78-0P
227276-79-1P 227276-81-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of carbamoylnaphthalenes as thrombin inhibitors)

RN 227276-66-6 CAPLUS

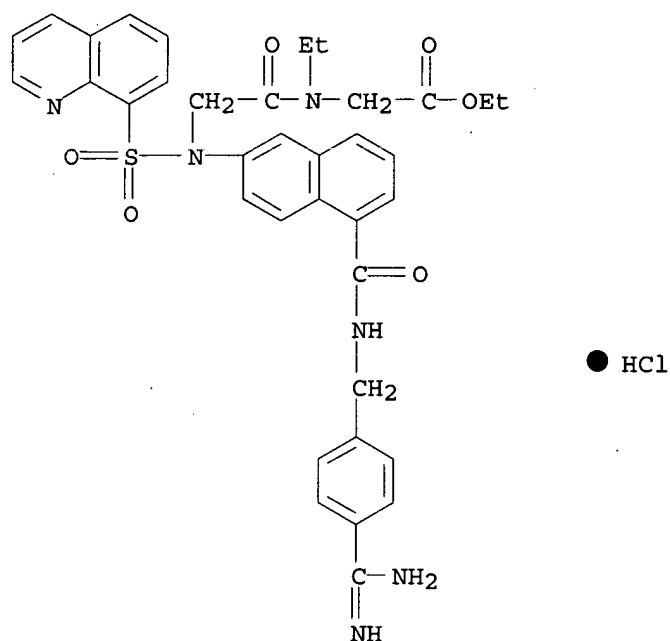
CN β -Alanine, N-[5-[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

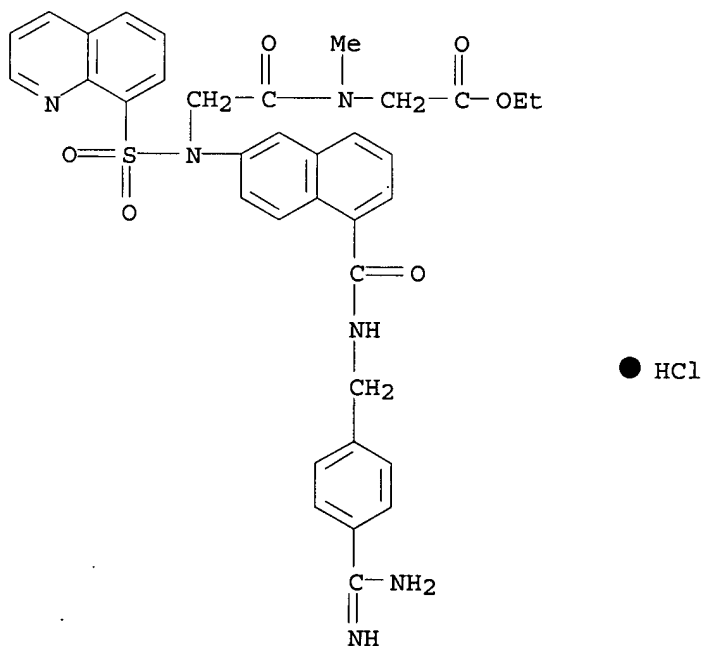
RN 227276-68-8 CAPLUS

CN Glycine, N-[5-[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-ethyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



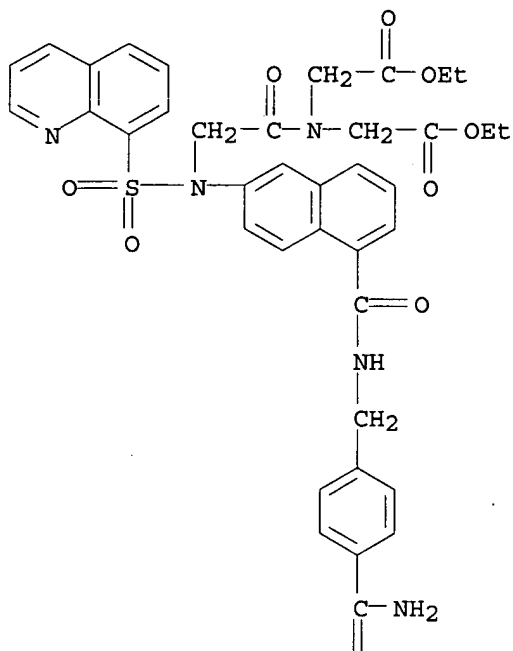
RN 227276-69-9 CAPLUS

CN Glycine, N-[5-[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



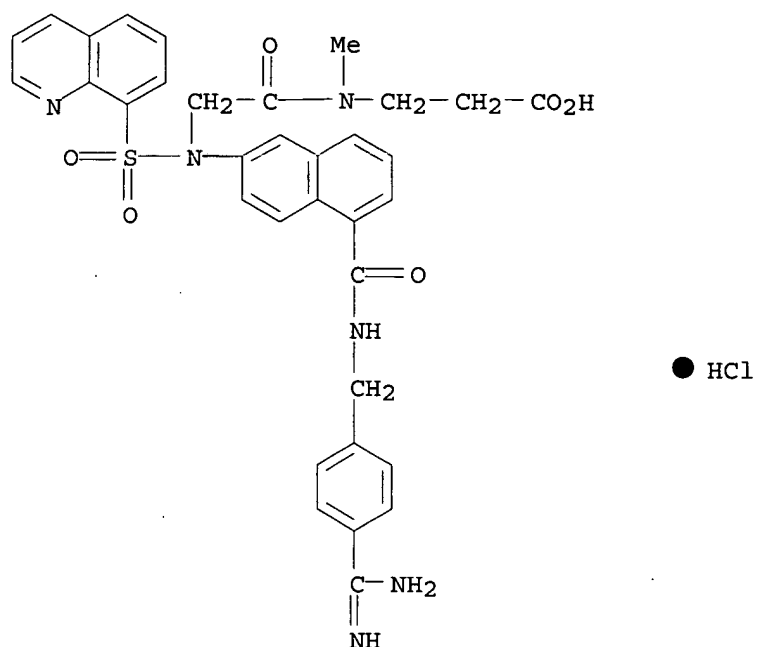
RN 227276-71-3 CAPLUS

CN Glycine, N-[5-[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-(2-ethoxy-2-oxoethyl)-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



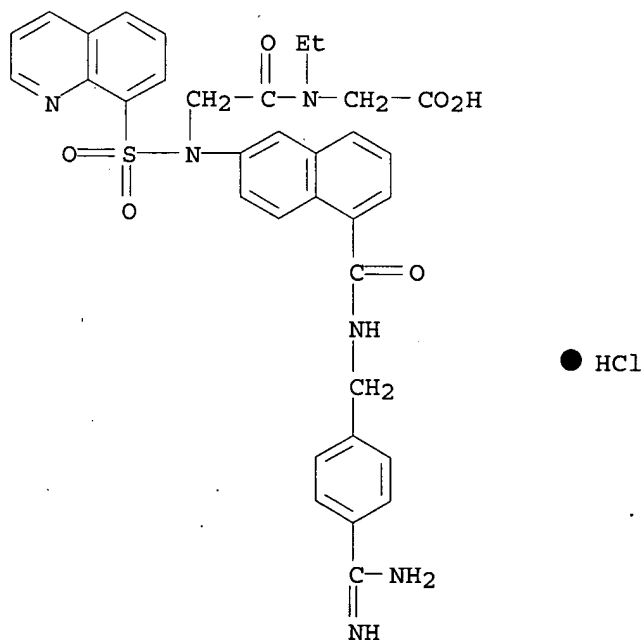
● HCl

RN 227276-76-8 CAPLUS
 CN β -Alanine, N-[5-[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-
 2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-,
 monohydrochloride (9CI) (CA INDEX NAME)



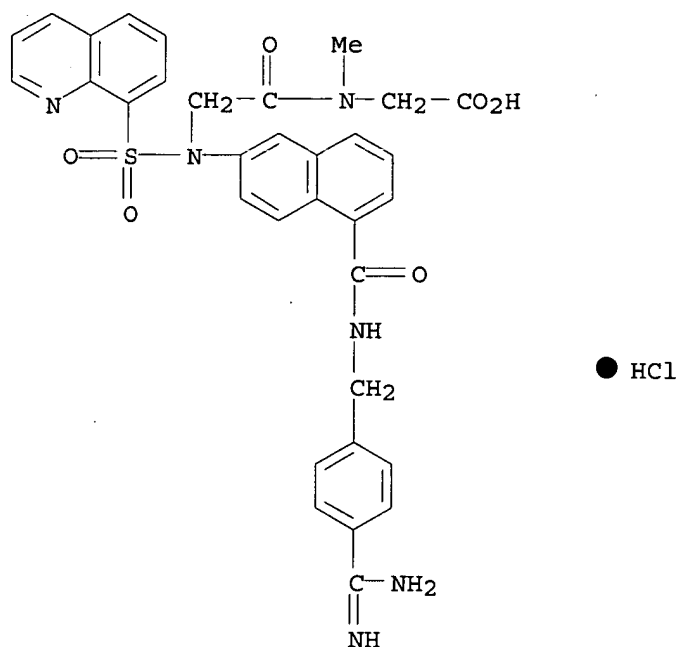
RN 227276-78-0 CAPLUS

CN Glycine, N-[5-[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)



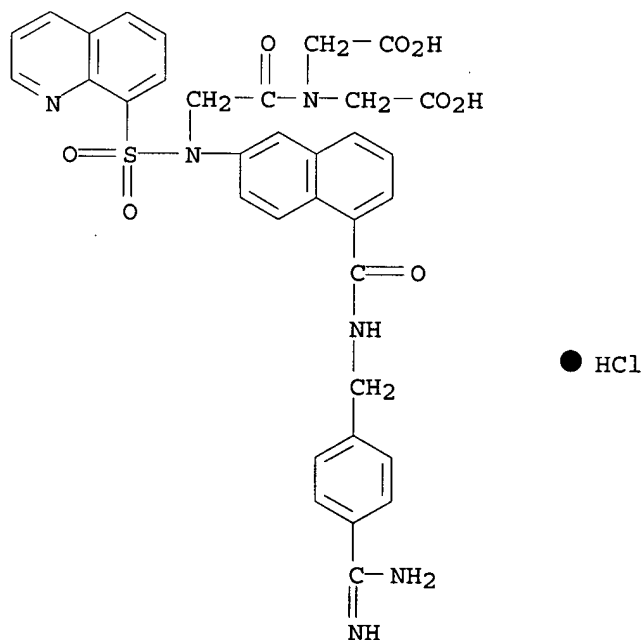
RN 227276-79-1 CAPLUS

CN Glycine, N-[5-[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



RN 227276-81-5 CAPLUS

CN Glycine, N-[5-[[[4-(aminoiminomethyl)phenyl]methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-(carboxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



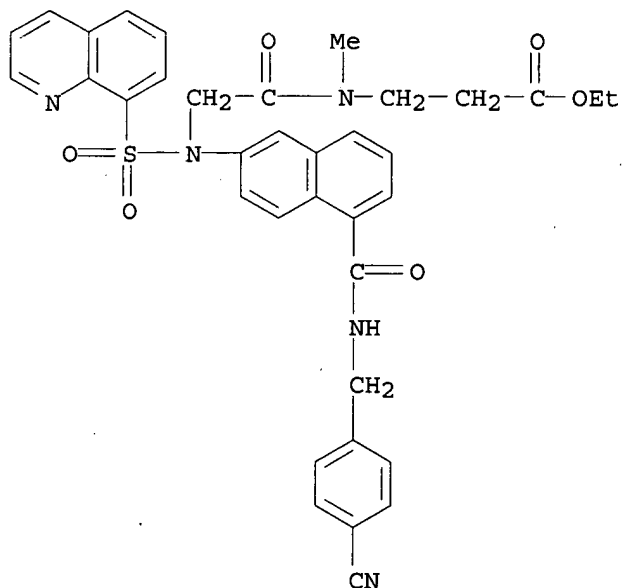
IT 227279-02-9 227279-04-1 227279-05-2
227279-07-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of carbamoylnaphthalenes as thrombin inhibitors)

RN 227279-02-9 CAPLUS

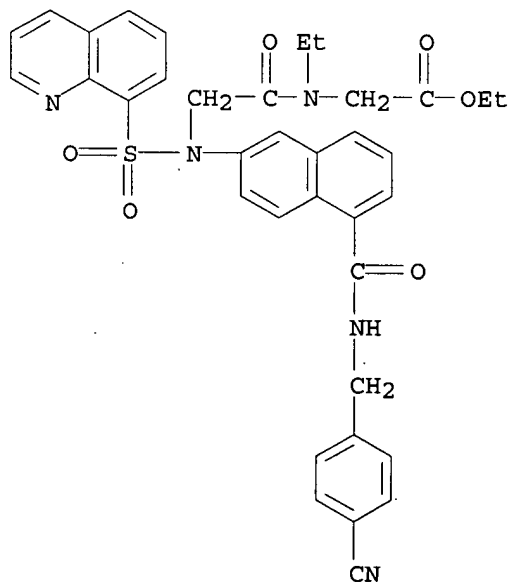
CN β-Alanine, N-[5-[[[4-(cyanophenyl)methyl]amino]carbonyl]-2-

naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester (9CI)
(CA INDEX NAME)



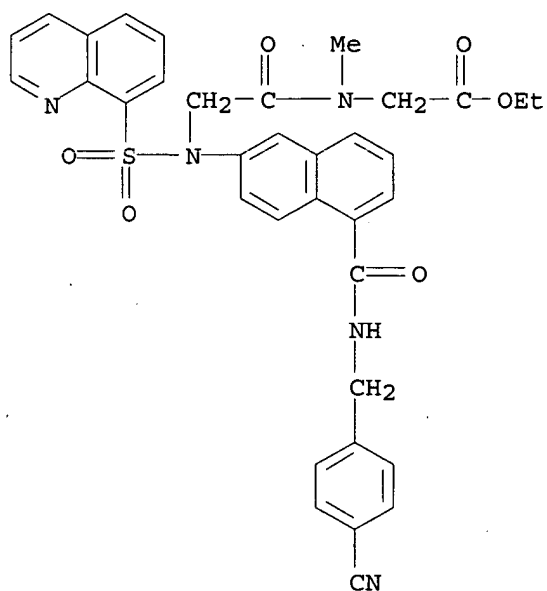
RN 227279-04-1 CAPLUS

CN Glycine, N-[5-[[[(4-cyanophenyl)methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-ethyl-, ethyl ester (9CI) (CA INDEX NAME)

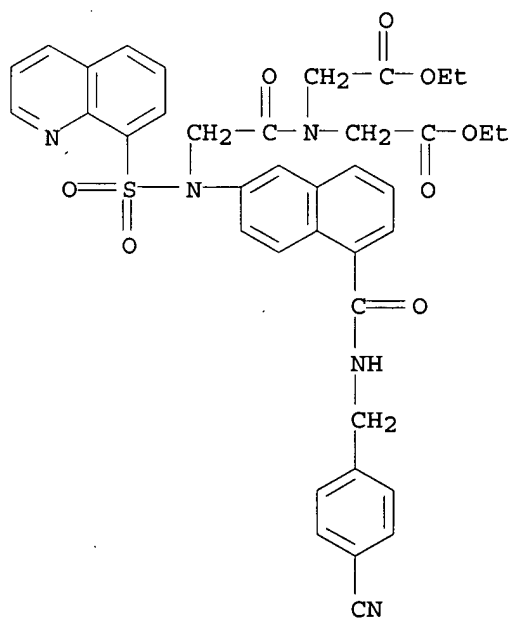


RN 227279-05-2 CAPLUS

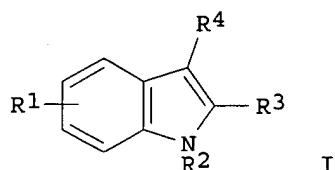
CN Glycine, N-[5-[[[(4-cyanophenyl)methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 227279-07-4. CAPLUS
 CN Glycine, N-[5-[[[(4-cyanophenyl)methyl]amino]carbonyl]-2-naphthalenyl]-N-(8-quinolinylsulfonyl)glycyl-N-(2-ethoxy-2-oxoethyl)-, ethyl ester (9CI)
 (CA INDEX NAME)



L6 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
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AB Title compds. [I; R1 = F, Cl, Br, CO₂H, aminocarbonyl, aminosulfonyl, amino, group convertible to CO₂H in vivo; 1 of R2, R4 = (CO₂H- or group convertible to CO₂H in vivo-substituted) alkyl, the other = R5A; A = (CO₂H- or group convertible to CO₂H in vivo-substituted) alkylene, etc.; R5 = R₆NHC(:NH)-substituted Ph; R4 = H, alkyl; R6 = H, in vivo-cleavable group], were prepared as antithrombotics with inhibitory activity against serine proteases XII and fibrinogen receptors. Thus, 3-[3-(4-amidinophenyl)propionyl]-1-methylindole-5-carboxylic acid N-(2-carboxyethyl)-N-phenylamide hydrochloride (preparation given) showed a thrombin time ED₂₀₀ = 0.80 μM.

ACCESSION NUMBER: 1999:375527 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 131:31874
TITLE: Preparation of amidinophenylpropionylindoles and related compounds as thrombin inhibitors.
INVENTOR(S): Heckel, Armin; Walter, Rainer; Soyka, Rainer; Stassen, Jean-Marie; Wienen, Wolfgang; Binder, Klaus
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma KG, Germany
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9928297	A1	19990610	WO 1998-EP7661	19981127
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
DE 19753522	A1	19990610	DE 1997-19753522	19971203
AU 9922671	A	19990616	AU 1999-22671	19981127
PRIORITY APPLN. INFO.:			DE 1997-19753522	A 19971203
			WO 1998-EP7661	W 19981127

OTHER SOURCE(S): MARPAT 131:31874

IT 226899-02-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

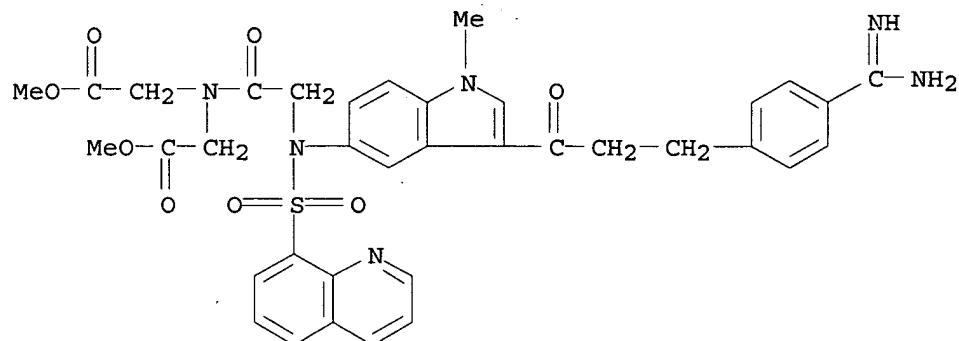
(preparation of amidinophenylpropionylindoles and related compds. as thrombin inhibitors)

RN 226899-02-1 CAPLUS

CN Glycine, N-[3-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-(2-methoxy-2-oxoethyl)-, methyl ester, monoacetate (9CI) (CA INDEX NAME)

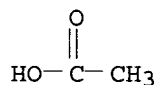
CM 1

CRN 226899-01-0
CMF C36 H36 N6 O8 S

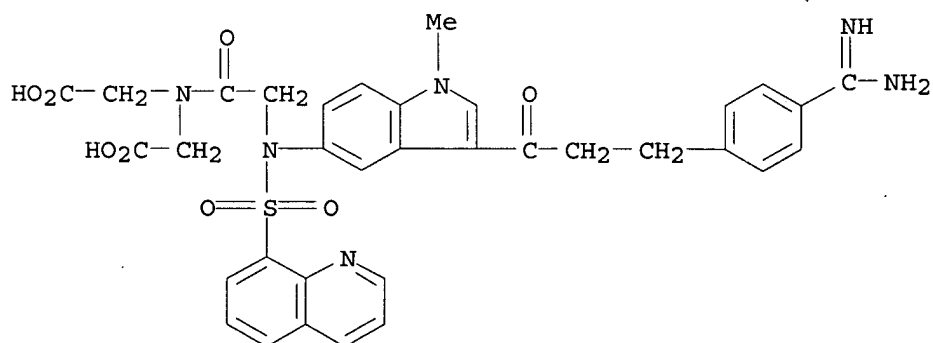


CM 2

CRN 64-19-7
CMF C2 H4 O2



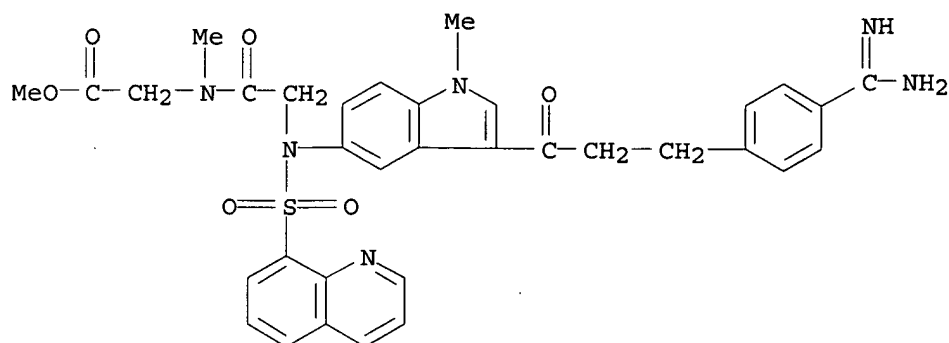
IT 226899-05-4P 226899-11-2P 226899-13-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidinophenylpropionylindoles and related compds. as thrombin inhibitors)
RN 226899-05-4 CAPLUS
CN Glycine, N-[3-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-(carboxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 226899-11-2 CAPLUS

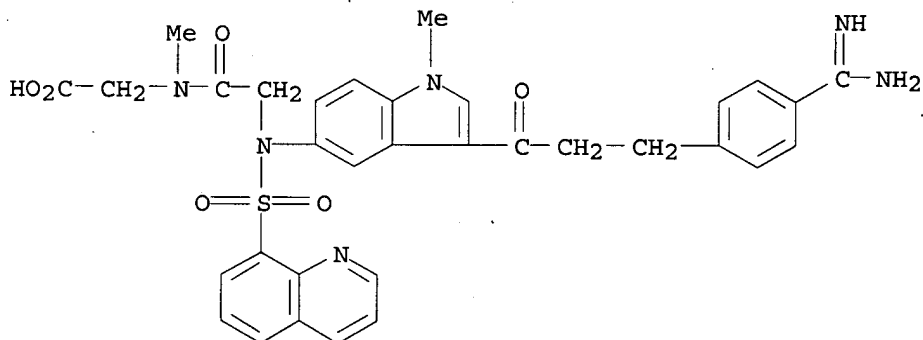
CN Glycine, N-[3-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, methyl ester, monohydriodide (9CI) (CA INDEX NAME)



● HI

RN 226899-13-4 CAPLUS

CN Glycine, N-[3-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)



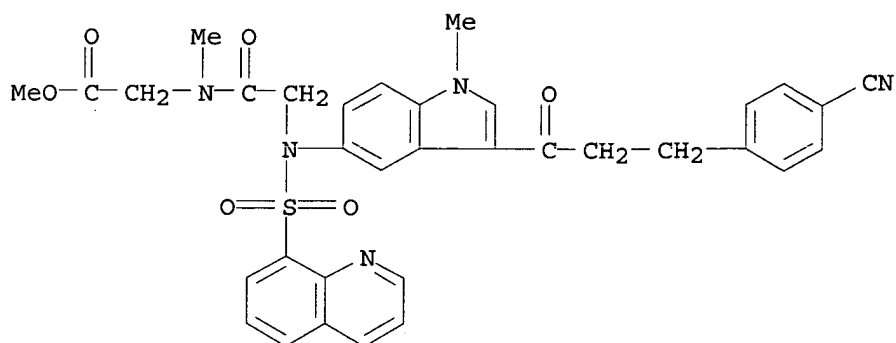
● HCl

IT 226902-20-1

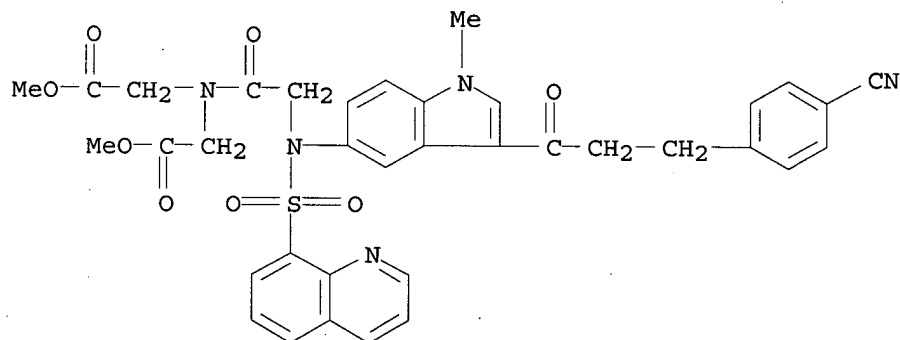
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amidinophenylpropionylindoles and related compds. as thrombin inhibitors)

RN 226902-20-1 CAPLUS

CN Glycine, N-[3-[3-(4-cyanophenyl)-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-methyl-, methyl ester (9CI) (CA INDEX NAME)

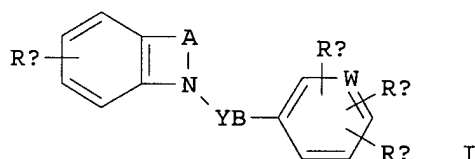


IT 226901-00-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of amidinophenylpropionylindoles and related compds. as thrombin inhibitors)
 RN 226901-00-4 CAPLUS
 CN Glycine, N-[3-[3-(4-cyanophenyl)-1-oxopropyl]-1-methyl-1H-indol-5-yl]-N-(8-quinolinylsulfonyl)glycyl-N-(2-methoxy-2-oxoethyl)-, methyl ester (9CI)
 (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 GI



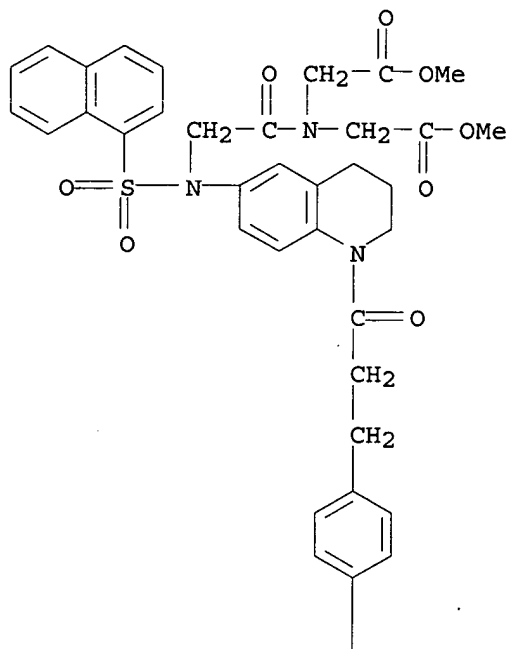
AB Title compds. [I; Ra = H, NO2, amino, aminocarbonyl; Rb = cyano, aminomethyl, (substituted) amidino; Rc, Rd = H, F, Cl, Br, iodo, Me, MeO, NO2, amino; A = (substituted) ethylene, ethenylene, propylene, etc.; B = bond, (substituted) methylene, ethylene, ethenylene, propylene, etc.; W =

N, CH; Y = CH₂, CO, CS], were prepared Thus, 1-[3-(4-amidinophenyl)propionyl]-1,2,3,4-tetrahydroquinoline-6-carboxylic acid methyl-N-phenylamide (preparation given) had a thrombin time ED200 = 0.02 µM.

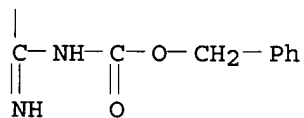
ACCESSION NUMBER: 1999:35065 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 130:110166
TITLE: Preparation of amidinophenylpropionyltetrahydroquinolines and related compounds as antithrombotics.
INVENTOR(S): Heckel, Armin; Soyka, Rainer; Grell, Wolfgang; Haaksma, Eric; Binder, Klaus; Zimmermann, Rainer
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany
SOURCE: Ger. Offen., 50 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19727117	A1	19990107	DE 1997-19727117	19970626
CA 2288744	A1	19990107	CA 1998-2288744	19980622
WO 9900371	A1	19990107	WO 1998-EP3800	19980622
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9887279	A	19990119	AU 1998-87279	19980622
EP 991624	A1	20000412	EP 1998-938621	19980622
EP 991624	B1	20031119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002511088	T	20020409	JP 1999-505265	19980622
AT 254602	T	20031215	AT 1998-938621	19980622
MX 9911261	A	20000630	MX 1999-11261	19991206
US 6300342	B1	20011009	US 1999-457961	19991209
PRIORITY APPLN. INFO.:			DE 1997-19727117	A 19970626
			WO 1998-EP3800	W 19980622
OTHER SOURCE(S): MARPAT 130:110166				
IT 219642-91-8P 219645-27-9P 219645-55-3P				
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)				
(preparation of amidinophenylpropionyltetrahydroquinolines and related compds. as antithrombotics)				
RN 219642-91-8 CAPLUS				
CN Glycine, N-(1-naphthalenylsulfonyl)-N-[1,2,3,4-tetrahydro-1-[3-[4-[imino[(phenylmethoxy)carbonyl]amino]methyl]phenyl]-1-oxopropyl]-6-quinolinyl]glycyl-N-(2-methoxy-2-oxoethyl)-, methyl ester (9CI) (CA INDEX NAME)				

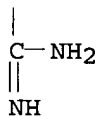
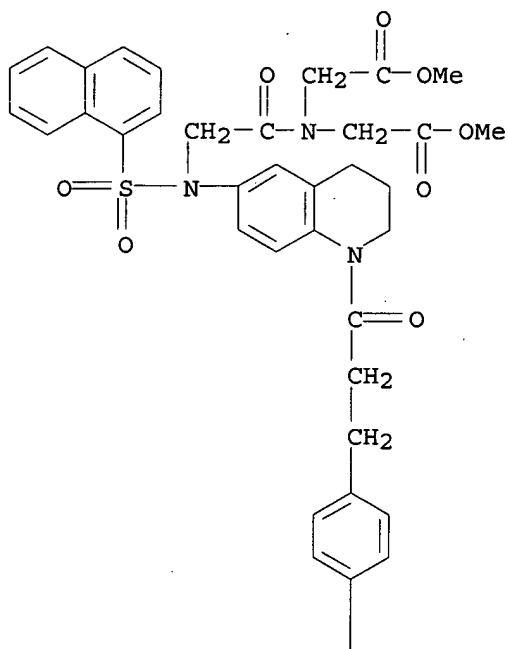
PAGE 1-A



PAGE 2-A

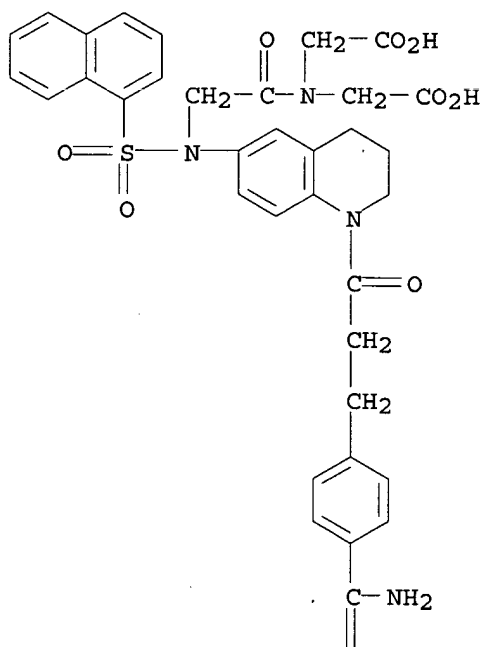


RN 219645-27-9 CAPLUS
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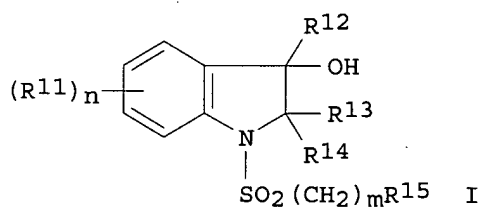
● HCl

RN 219645-55-3 CAPLUS
 CN Glycine, N-[1-[3-[4-(aminoiminomethyl)phenyl]-1-oxopropyl]-1,2,3,4-tetrahydro-6-quinolinyl]-N-(1-naphthalenylsulfonyl)glycyl-N-(carboxymethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L6 ANSWER 8. OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
GI



AB Title compds. I (R'1 = halo, C1-4 alkyl, HO, C1-4 alkoxy, PhCH2O, NC, F3C, O2N, H2N; R'2 = C1-6 alkyl, C3-7 cycloalkyl, C5-7 cycloalkylene, (substituted) Ph, etc.; R'3 = H; R'4 = H2NCO, R'6R'7NCO wherein R'6R'7N = saturated 5-membered substituted N-heterocyclyl; R'5 = C1-4 alkyl, 1-, 2-naphthyl, (substituted) Ph, etc.; n = m = 0-2) or a salt thereof, are prepared CH2BrCONMe2 (preparation given) and 5-chloro-2-(tosylamino)phenyl cyclohexyl ketone were reacted to give

2-[N-tosyl-N-(dimethylcarbamoylmethyl)amino]-5-(chlorophenyl) cyclohexyl ketone which in THF was treated with Li diisopropylamide to give after workup trans-I (R'1n = 5-Cl, R'2 = cyclohexyl, R'3 = H, R'4 = Me2NCO, R'5 = 4-MeC6H4, m = 0). The IC50 of I affinity for oxytocin receptors was 10-5-10-8M.

ACCESSION NUMBER: 1995:777639 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER: 123:198616
TITLE: Preparation of N-sulfonylindoline derivatives with affinity for vasopressin and oxytocin receptors
INVENTOR(S): Wagnon, Jean; de Cointet, Paul; Nisato, Dino; Plouzane, Claude; Sereadeil-Legal, Claudine; Tonnerre, Bernard
PATENT ASSIGNEE(S): Elf Sanofi SA, Fr.
SOURCE: U.S., 50 pp. Cont.-in-part of U.S. Ser. No.737,655, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5338755	A	19940816	US 1992-923839	19920803
FR 2665441	A1	19920207	FR 1990-9778	19900731
FR 2665441	B1	19921204		
IL 114934	A	19960804	IL 1991-114934	19910730
HU 219351	B	20010328	HU 1971-99045	19910731
FR 2679903	A1	19930205	FR 1991-9908	19910802
FR 2679903	B1	19931203		
AU 9224758	A	19930302	AU 1992-24758	19920731
AU 658664	B2	19950427		
BR 9205336	A	19931116	BR 1992-5336	19920731
JP 06501960	T	19940303	JP 1993-503337	19920731
RU 2104268	C1	19980210	RU 1993-5168	19920731
IL 117592	A	19990411	IL 1992-117592	19920731
CZ 288173	B6	20010516	CZ 1993-682	19920731
CA 2206776	C	20020226	CA 1992-2206776	19920731
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NO 9301262	A	19930526	NO 1993-1262	19930401
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US 5397801	A	19950314	US 1994-240360	19940510
US 5481005	A	19960102	US 1994-348150	19941128
US 5578633	A	19961126	US 1995-458614	19950602
FI 9800175	A	19980127	FI 1998-175	19980127
FI 107048	B1	20010531		

PRIORITY APPLN. INFO.:

FR 1990-9778	A	19900731
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CA 1992-2093221	A3	19920731
CS 1993-682	A	19920731
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OTHER SOURCE(S): MARPAT 123:198616

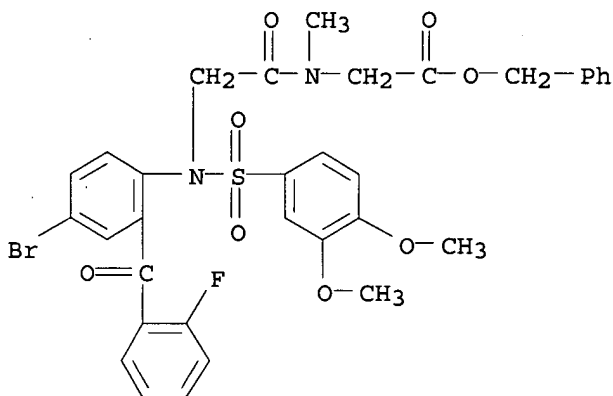
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 149152-36-3P 149152-39-6P 149152-40-9P
 149152-42-1P 149152-43-2P 149152-44-3P
 167400-68-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-sulfonylindoline derivs. with affinity for vasopressin and oxytocin receptors)

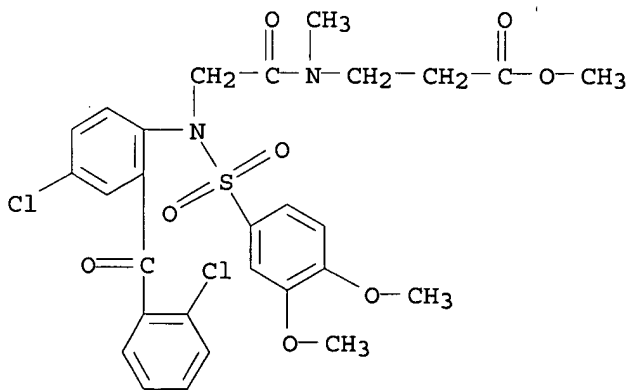
RN 149152-33-0 CAPLUS

CN Glycine, N- [N- [4-bromo-2- (2-fluorobenzoyl)phenyl] -N- [(3,4-dimethoxyphenyl)sulfonyl]glycyl] -N-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)



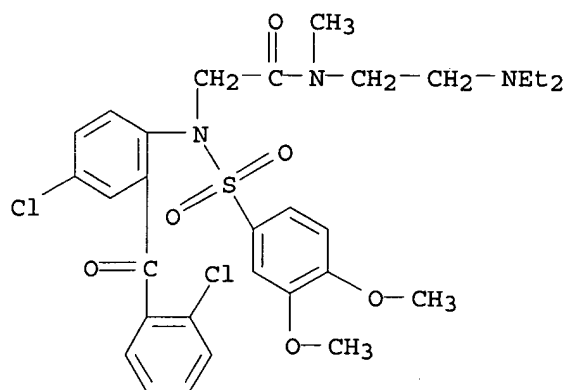
RN 149152-34-1 CAPLUS

CN β -Alanine, N- [N- [4-chloro-2- (2-chlorobenzoyl)phenyl] -N- [(3,4-dimethoxyphenyl)sulfonyl]glycyl] -N-methyl-, methyl ester (9CI) (CA INDEX NAME)



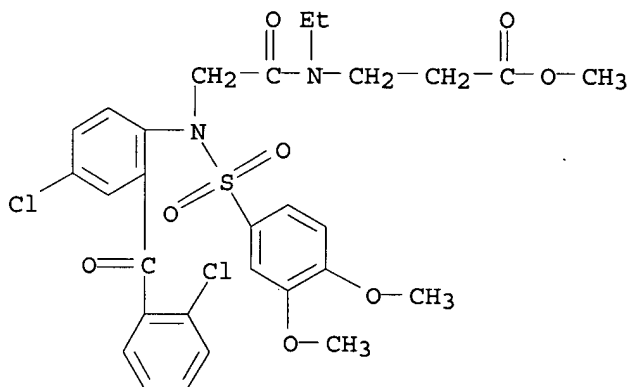
RN 149152-35-2 CAPLUS

CN Acetamide, 2- [[4-chloro-2- (2-chlorobenzoyl)phenyl] [(3,4-dimethoxyphenyl)sulfonyl]amino] -N- [2- (diethylamino)ethyl] -N-methyl- (9CI) (CA INDEX NAME)



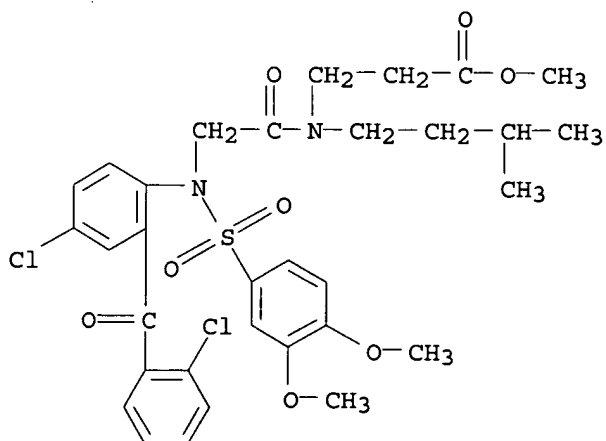
RN 149152-36-3 CAPLUS

CN β -Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)

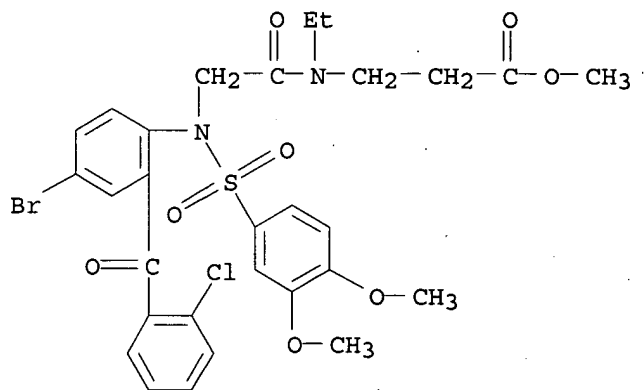


RN 149152-39-6 CAPLUS

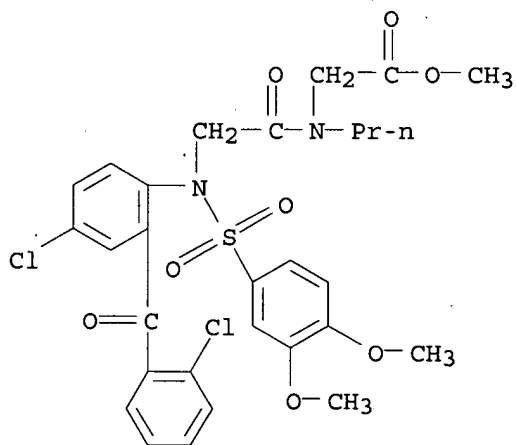
CN β -Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(3-methylbutyl)-, methyl ester (9CI) (CA INDEX NAME)



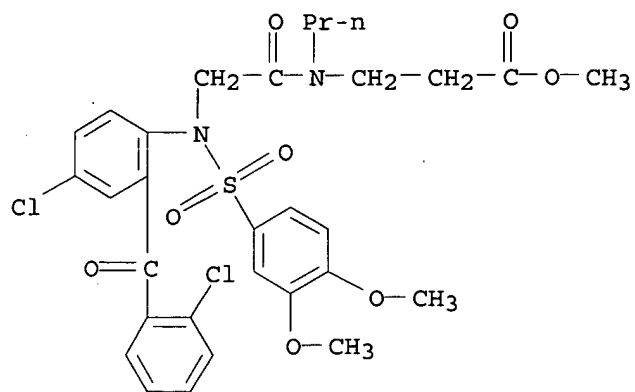
RN 149152-40-9 CAPLUS
 CN β -Alanine, N-[N-[4-bromo-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



RN 149152-42-1 CAPLUS
 CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-propyl-, methyl ester (9CI) (CA INDEX NAME)

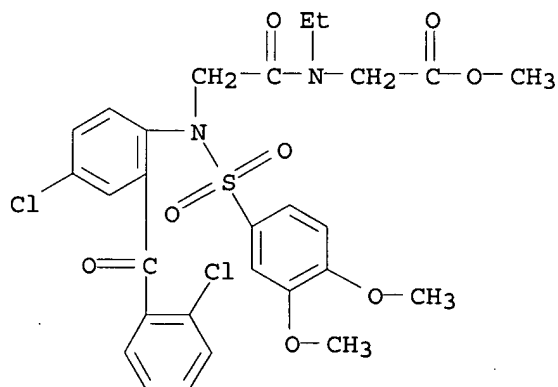


RN 149152-43-2 CAPLUS
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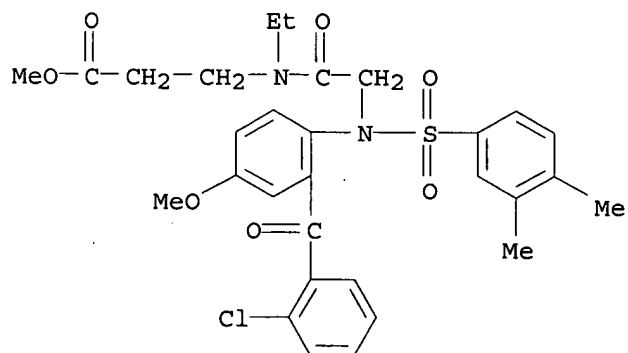
RN 149152-44-3 CAPLUS

CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



RN 167400-68-2 CAPLUS

CN β -Alanine, N-[N-[2-(2-chlorobenzoyl)-4-methoxyphenyl]-N-[(3,4-dimethylphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



IT 149152-22-7P 149152-26-1P 149152-31-8P
149152-48-7P 149152-51-2P 167400-91-1P

167400-95-5P

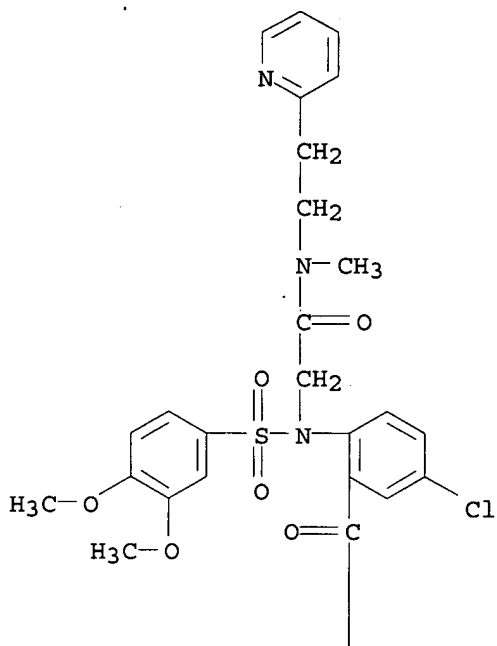
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-sulfonylindoline derivs. with affinity for vasopressin and oxytocin receptors)

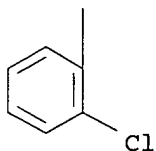
RN 149152-22-7 CAPLUS

CN Acetamide, 2-[[4-chloro-2-(2-chlorobenzoyl)phenyl][(3,4-dimethoxyphenyl)sulfonyl]amino]-N-methyl-N-[2-(2-pyridinyl)ethyl]- (9CI)
(CA INDEX NAME)

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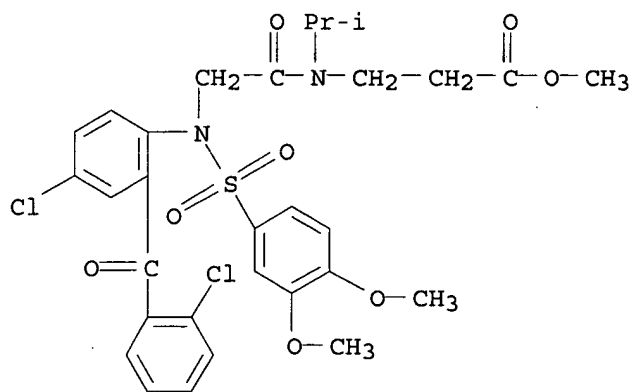


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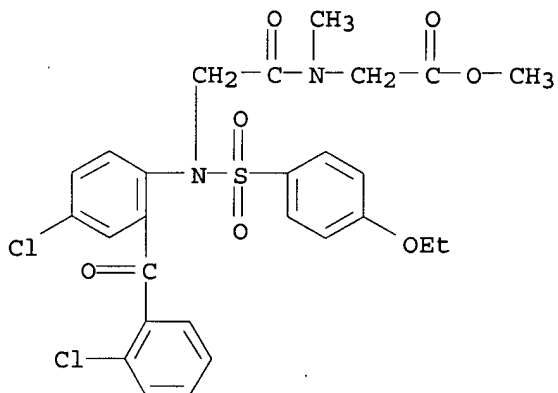
RN 149152-26-1 CAPLUS

CN β -Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(1-methylethyl)-, methyl ester (9CI)
(CA INDEX NAME)



RN 149152-31-8 CAPLUS

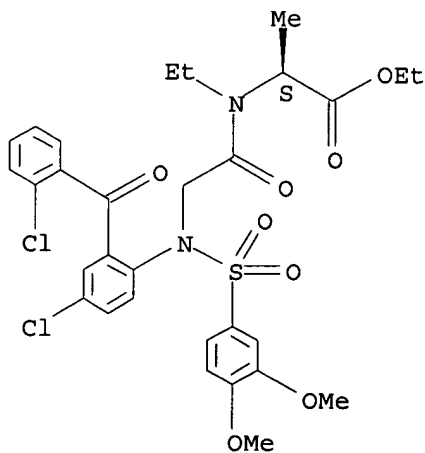
CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(4-ethoxyphenyl)sulfonyl]glycyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



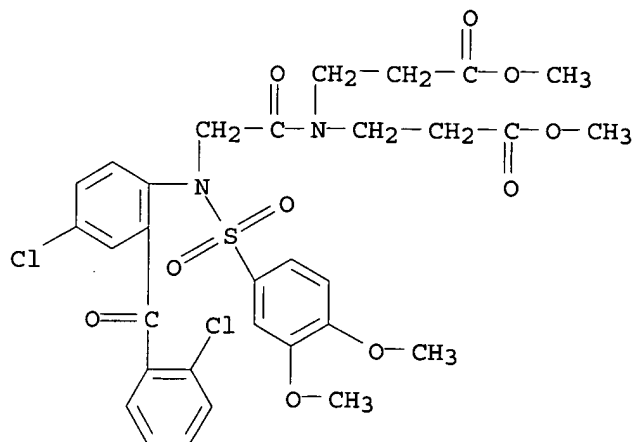
RN 149152-48-7 CAPLUS

CN L-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, ethyl ester (9CI) (CA INDEX NAME)

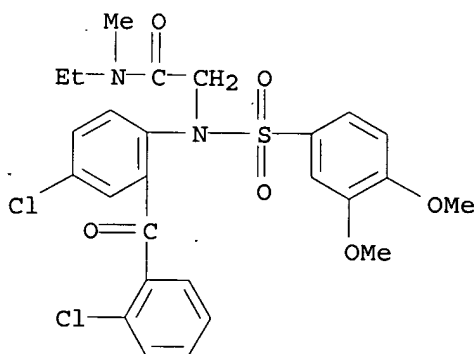
Absolute stereochemistry.



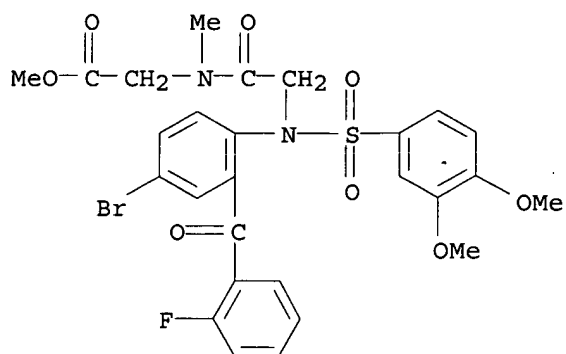
RN 149152-51-2 CAPLUS
 CN β -Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(3-methoxy-3-oxopropyl)-, methyl ester (9CI) (CA INDEX NAME)



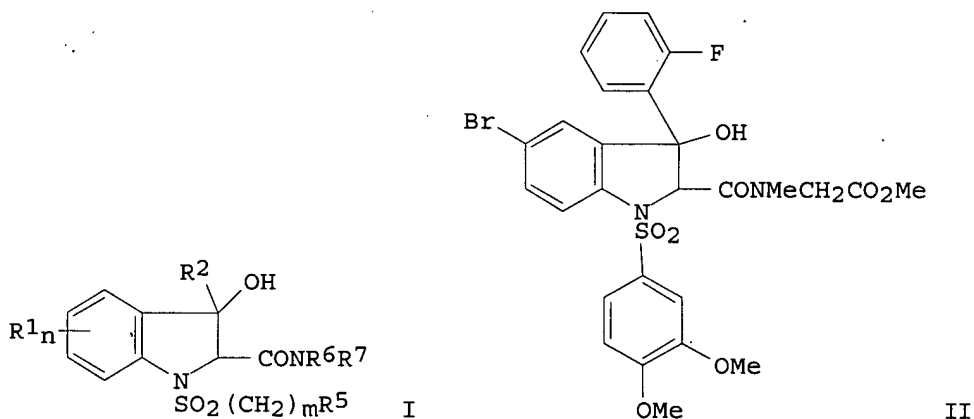
RN 167400-91-1 CAPLUS
 CN Acetamide, 2-[[4-chloro-2-(2-chlorobenzoyl)phenyl][(3,4-dimethoxyphenyl)sulfonyl]amino]-N-ethyl-N-methyl- (9CI) (CA INDEX NAME)



RN 167400-95-5 CAPLUS
 CN Glycine, N-[N-[4-bromo-2-(2-fluorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



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AB Title compds. [I; R1 = OH, halo, alkyl, alkoxy, etc.; R2 = (cyclo)alkyl, (nitro)phenyl, etc.; R5 = alkyl, (nitro)phenyl, naphthyl, etc.; R6 = alkyl; R6, R7 = 4-piperidinyl, 3-azetidiny, etc.; NR6R7 = (thio)morpholino, thiazolidino, piperazino, etc.; m, n = 0-2] were prepared. Thus, 2-amino-5-bromo-2'-fluorobenzophenone was amidated by 3,4-(MeO)2C6H3SO2Cl and the product N-alkylated by BrCH2CONMeCH2CO2Me to give, after cyclization of the product, title compound II. I had IC50 of 10-9, and 10-5 to 10-8 M, against vasopressin and oxytocin binding, resp., in vitro.

ACCESSION NUMBER:	1993:539091 CAPLUS <<LOGINID::20070131>>
DOCUMENT NUMBER:	119:139091
TITLE:	Preparation of 1-phenylsulfonyl-3-hydroxyindoline-2-carboxamides as oxytocin and vasopressin antagonists
INVENTOR(S):	Wagnon, Jean; Serradeil-Legal, Claudine; Tonnerre, Bernard; Plouzane, Claude; Nisato, Dino
PATENT ASSIGNEE(S):	Elf Sanofi SA, Fr.
SOURCE:	Eur. Pat. Appl., 71 pp.
	CODEN: EPXXDW
DOCUMENT TYPE:	Patent
LANGUAGE:	French
FAMILY ACC. NUM. COUNT:	3
PATENT INFORMATION:	

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 526348	A1	19930203	EP 1992-402213	19920803
EP 526348	B1	19980218		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
FR 2679903	A1	19930205	FR 1991-9908	19910802
FR 2679903	B1	19931203		
CA 2093221	A1	19930203	CA 1992-2093221	19920731
CA 2093221	C	19980922		
WO 9303013	A1	19930218	WO 1992-FR758	19920731
W: AU, BR, CA, CS, FI, HU, JP, KR, NO, RU				
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AU 658664	B2	19950427		
ZA 9205781	A	19930302	ZA 1992-5781	19920731
BR 9205336	A	19931116	BR 1992-5336	19920731
JP 06501960	T	19940303	JP 1993-503337	19920731
LT 3064	B	19941025	LT 1992-114	19920731
LV 10091	B	19950420	LV 1992-87	19920731
HU 68927	A2	19950828	HU 1993-951	19920731
IL 102703	A	19970318	IL 1992-102703	19920731
JP 2633085	B2	19970723	JP 1992-503337	19920731
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US 5481005	A	19960102	US 1994-348150	19941128
AU 9511541	A	19950504	AU 1995-11541	19950203
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PRIORITY APPLN. INFO.:

FR 1991-9908	A	19910802
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US 1991-737655	B2	19910730
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IL 1992-102703	A3	19920731
WO 1992-FR758	A	19920731
FI 1993-1476	A	19930401
US 1993-923839	A3	19930803
US 1994-240360	A3	19940510

OTHER SOURCE(S): MARPAT 119:139091

IT 149152-22-7P 149152-26-1P 149152-31-8P
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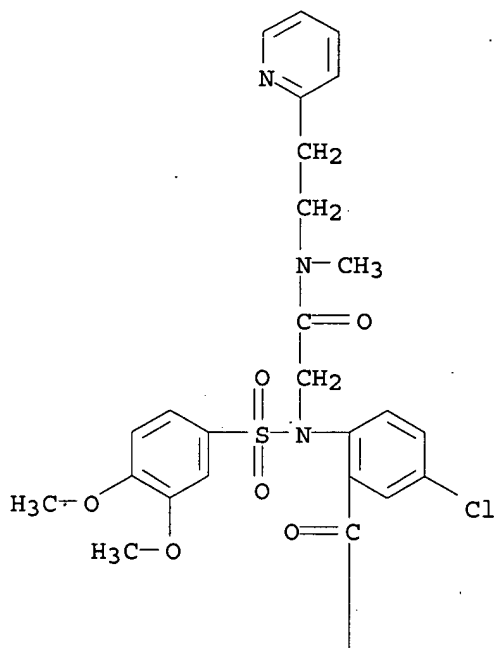
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of oxytocin and vasopressin antagonists)

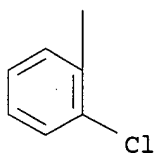
RN 149152-22-7 CAPLUS

CN Acetamide, 2-[[4-chloro-2-(2-chlorobenzoyl)phenyl][(3,4-dimethoxyphenyl)sulfonyl]amino]-N-methyl-N-[2-(2-pyridinyl)ethyl]- (9CI)
 (CA INDEX NAME)

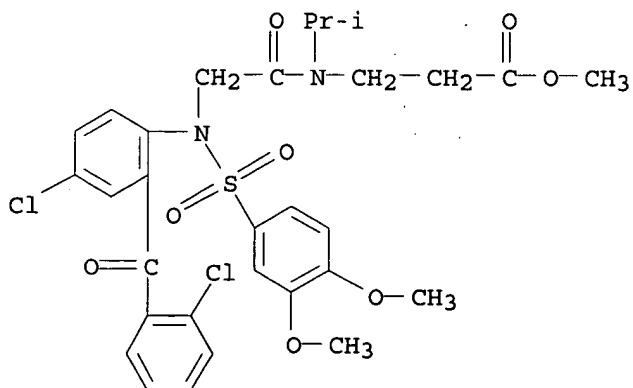
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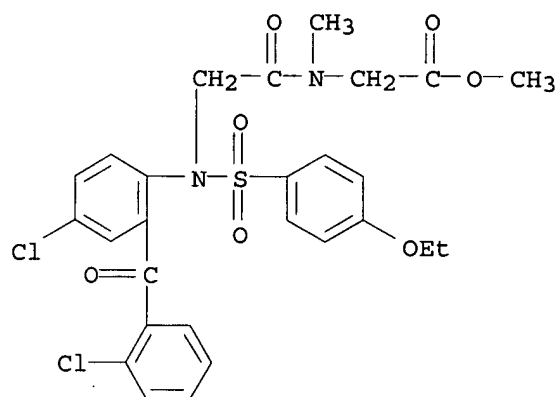


RN 149152-26-1 CAPLUS
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 (CA INDEX NAME)



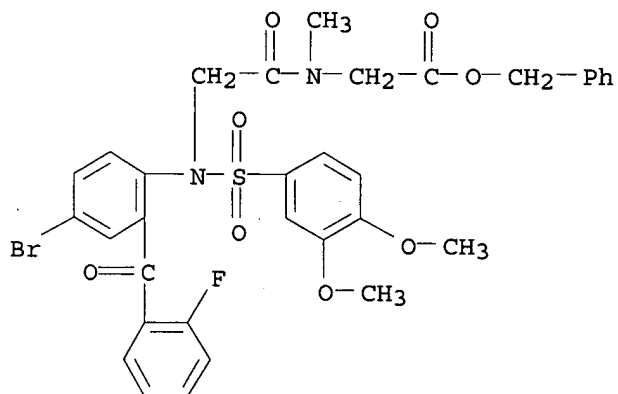
RN 149152-31-8 CAPLUS

CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(4-ethoxyphenyl)sulfonyl]glycyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



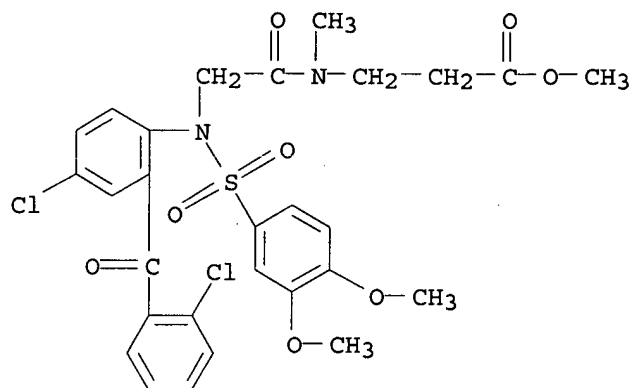
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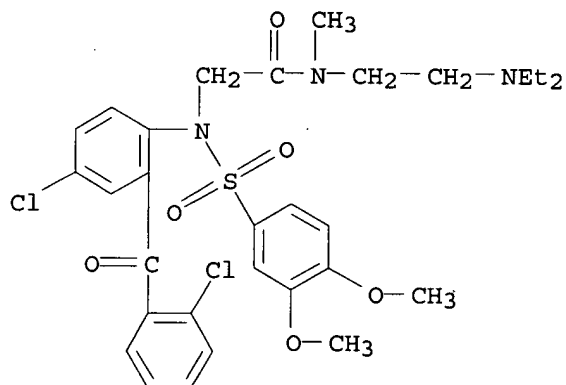


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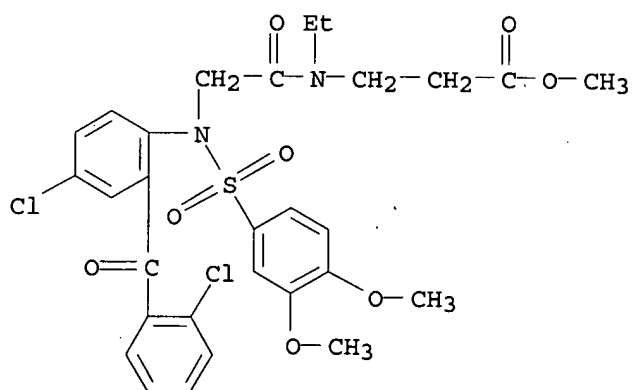
CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-methyl-, methyl ester (9CI) (CA INDEX NAME)



RN 149152-35-2 CAPLUS
 CN Acetamide, 2-[[4-chloro-2-(2-chlorobenzoyl)phenyl] [(3,4-dimethoxyphenyl)sulfonyl]amino]-N-[2-(diethylamino)ethyl]-N-methyl- (9CI)
 (CA INDEX NAME)

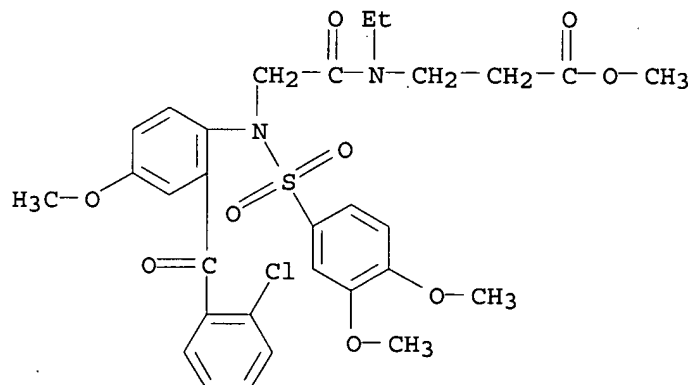


RN 149152-36-3 CAPLUS
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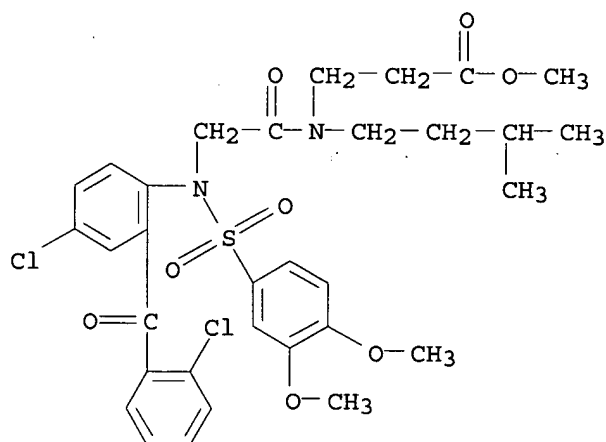


RN 149152-38-5 CAPLUS

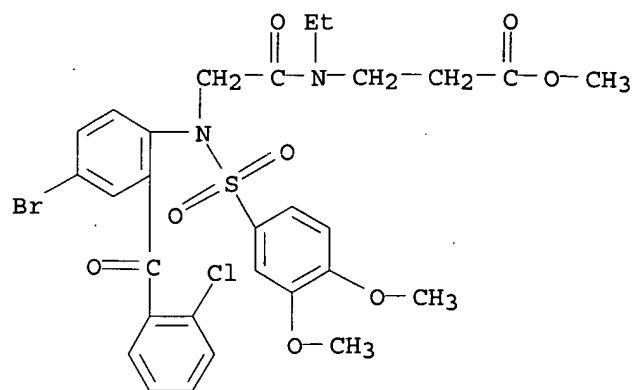
CN β -Alanine, N-[N-[2-(2-chlorobenzoyl)-4-methoxyphenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



RN 149152-39-6 CAPLUS
CN β -Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(3-methylbutyl)-, methyl ester (9CI) (CA INDEX NAME)

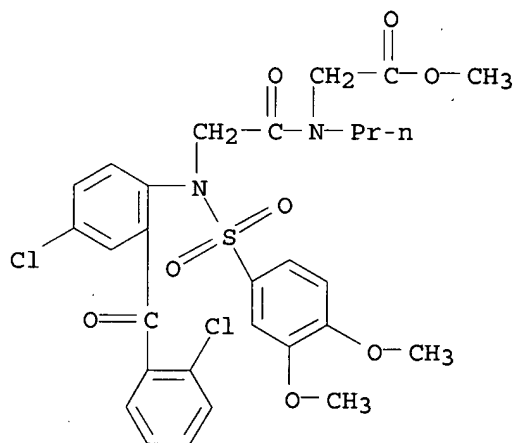


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CN β -Alanine, N-[N-[4-bromo-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



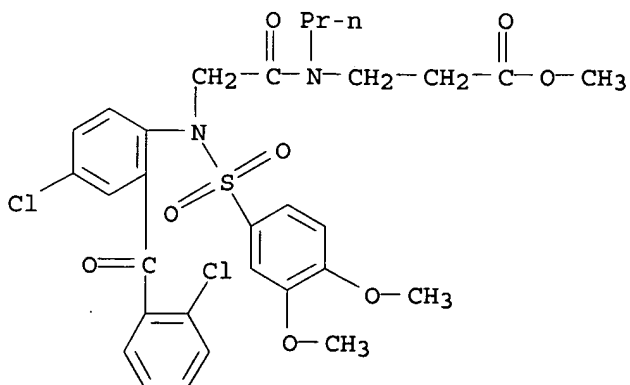
RN 149152-42-1 CAPLUS

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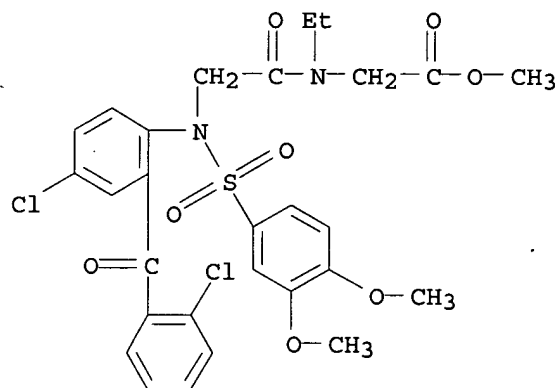
RN 149152-43-2 CAPLUS

CN β -Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-propyl-, methyl ester (9CI) (CA INDEX NAME)



RN 149152-44-3 CAPLUS

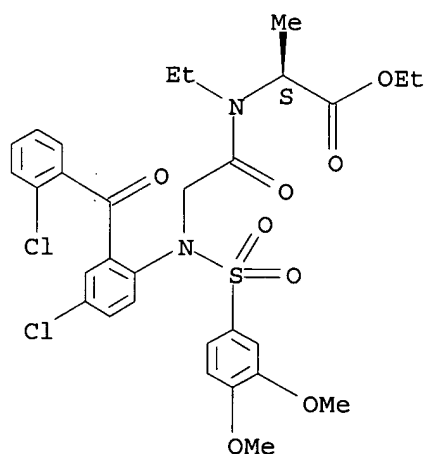
CN Glycine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, methyl ester (9CI) (CA INDEX NAME)



RN 149152-48-7 CAPLUS

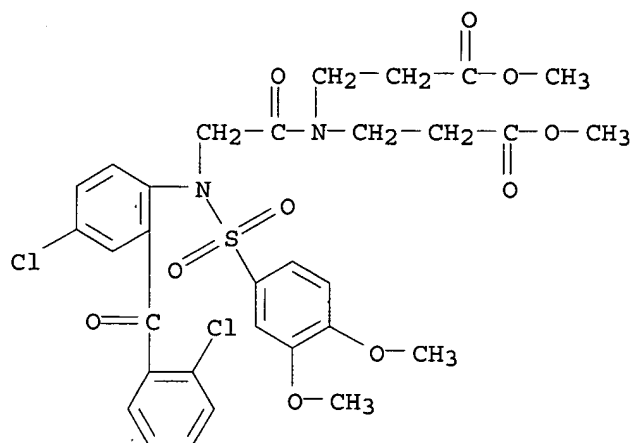
CN L-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-ethyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 149152-51-2 CAPLUS

CN β-Alanine, N-[N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-[(3,4-dimethoxyphenyl)sulfonyl]glycyl]-N-(3-methoxy-3-oxopropyl)-, methyl ester (9CI) (CA INDEX NAME)

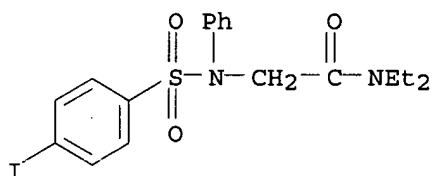


L6 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN
 AB RSO₂NHR' in aqueous NaOH (50% excess), treated with an equimolar amount of R''₂NCSCl at 5° and the mixture stirred 2 hrs. at 20° gave the following RSO₂NR'CSNR''₂ (% yield, R, R', R'', and m.p. shown): 54.2, Me, Ph, Me, 119-20°; 85.3, Et, Ph, Me, 101-2°; 87.1, Et, p-NCSC₆H₄, Et, 103-4°; 91.5, Ph, Ph, Me, 152-3°; 65.5, p-MeC₆H₄, p-ClC₆H₄, Me, 136-6.5°; 85.5, o-MeC₆H₄, Ph, Me, 124.5-5°; 86.3, iso-Pr, Ph, Et, 113-14°; 64.5, p-MeC₆H₄, Cl, Me, 149-50°; 91.6, p-FC₆H₄, Ph, Me, 151-2°; 62.7, p-ClC₆H₄, Ph, Me, 161-2°; 78.5, p-BrC₆H₄, Ph, Me, 154-5°; 52.7, p-IC₆H₄, Ph, Me, 156-7°. The p-iodophenyl member was prepared in Me₂CO. Heating p-MeC₆H₄SO₂NPhCSNMe₂ with 40% H₂SO₄, 46 hrs. at 150° gave CSO, PhNH₂, and Me₂NH, as well as p-MeC₆H₄SO₃H.

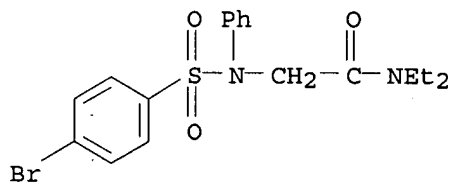
ACCESSION NUMBER: 1963:33089 CAPLUS <<LOGINID::20070131>>
 DOCUMENT NUMBER: 58:33089
 ORIGINAL REFERENCE NO.: 58:5567d-e
 TITLE: Sulfanilides. II. N-Sulfonyl derivatives of urea
 AUTHOR(S): Malinovskii, M. S.; Solomko, Z. F.; Glushko, L. P.
 CORPORATE SOURCE: State Univ., Dnepropetrovsk
 SOURCE: Zhurnal Obshchei Khimii (1962), 32, 728-31
 CODEN: ZOKHA4; ISSN: 0044-460X
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable

IT 88784-29-6P, Acetamide, N,N-diethyl-2-(p-iodo-N-phenylbenzenesulfonamido) - 93904-37-1P, Acetamide, 2-(p-bromo-N-phenylbenzenesulfonamido)-N,N-diethyl- 93995-09-6P, Acetamide, 2-(p-chloro-N-phenylbenzenesulfonamido)-N,N-diethyl- 93996-27-1P, Acetamide, N,N-diethyl-2-(p-nitro-N-phenylbenzenesulfonamido) - 94437-71-5P, Acetamide, N,N-diethyl-2-(N-phenyl-p-toluenesulfonamido) - 95167-60-5P, Acetamide, N,N-diethyl-2-(m-nitro-N-phenylbenzenesulfonamido) - 98981-10-3P, Acetamide, 2-(p-chloro-N-m-tolylbenzenesulfonamido) - N,N-diethyl-
 RL: PREP (Preparation)
 (preparation of)

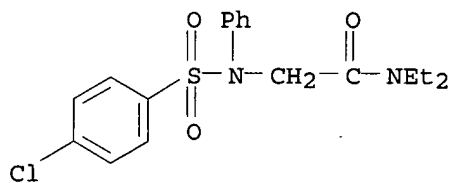
RN 88784-29-6 CAPLUS
 CN Acetamide, N,N-diethyl-2-(p-iodo-N-phenylbenzenesulfonamido) - (7CI) (CA INDEX NAME)



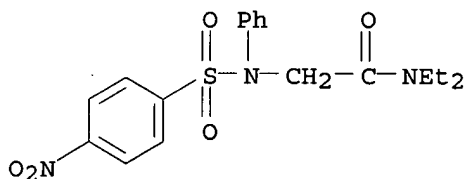
RN 93904-37-1 CAPLUS
 CN Acetamide, 2-(p-bromo-N-phenylbenzenesulfonamido)-N,N-diethyl- (7CI) (CA INDEX NAME)



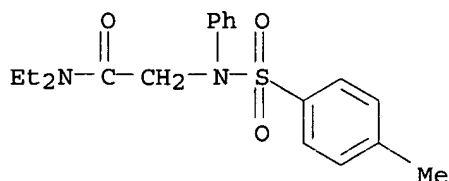
RN 93995-09-6 CAPLUS
 CN Acetamide, 2-(p-chloro-N-phenylbenzenesulfonamido)-N,N-diethyl- (7CI) (CA INDEX NAME)



RN 93996-27-1 CAPLUS
 CN Acetamide, N,N-diethyl-2-(p-nitro-N-phenylbenzenesulfonamido)- (7CI) (CA INDEX NAME)

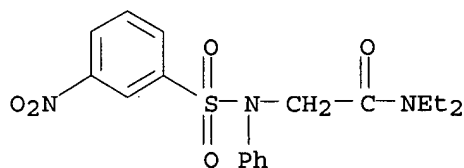


RN 94437-71-5 CAPLUS
 CN Acetamide, N,N-diethyl-2-(N-phenyl-p-toluenesulfonamido)- (7CI) (CA INDEX NAME)



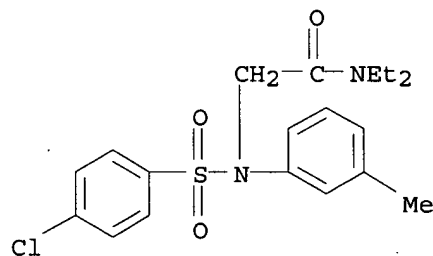
RN 95167-60-5 CAPLUS

CN Acetamide, N,N-diethyl-2-(m-nitro-N-phenylbenzenesulfonamido)- (7CI) (CA INDEX NAME)



RN 98981-10-3 CAPLUS

CN Acetamide, 2-(p-chloro-N-m-tolylbenzenesulfonamido)-N,N-diethyl- (7CI) (CA INDEX NAME)



L6 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

AB Addition of RSO₂NHAr to aqueous NaOH (equimolar amount), followed by ClCH₂CONEt₂

in EtOH and 2-4 hrs. refluxing gave the following RSO₂NArCH₂CONEt₂ (R, Ar, % yield and m.p. shown): Me, Ph, 60.6, 97-8°; Et, Ph, 57, 80-1°; Ph, Ph (I), 91.5, 93-4°; p-ClC₆H₄, Ph, 58, 117-18°; p-BrC₆H₄, Ph, 65.2, 102.5-3°; p-IC₆H₄, Ph, 44.5, 150.5-1°; p-ClC₆H₄, m-MeC₆H₄, 80.5, 77-8°; p-O₂NC₆H₄, Ph, 46.5, 148-8.5° m-O₂NC₆H₄, Ph, 72.3, 134-4.5°; p-MeC₆H₄, Ph, 95, 128-9° Heating PhNH₂ with ClCH₂CONEt₂ in BuOH in the presence of Na₂CO₃ 8-10 hrs. gave 39.2% PhNHCH₂CONEt₂, b₄ 175-82° (U.S. 2,568,142, CA 46, 3568a), which, heated with NaOAc in 30% EtOH to 70°, and treated with PhSO₂Cl over 1 hr. gave I.

ACCESSION NUMBER: 1963:33088 CAPLUS <<LOGINID::20070131>>

DOCUMENT NUMBER: 58:33088

ORIGINAL REFERENCE NO.: 58:5567c-d

TITLE: Sulfanilides. I. N-Sulfonylarylglycine dialkylamides

AUTHOR(S): Malinovskii, M. S.; Solomko, Z. F.; Teslenko, E. P.; Efremova, A. L.

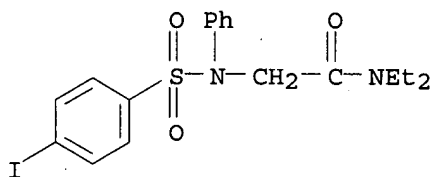
CORPORATE SOURCE: State Univ., Dnepropetrovsk

SOURCE: Zhurnal Obshchei Khimii (1962), 32, 726-8

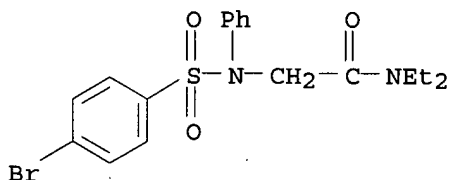
CODEN: ZOKHAA; ISSN: 0044-460X

DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

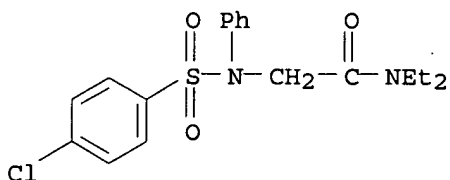
IT 88784-29-6P, Acetamide, N,N-diethyl-2-(p-iodo-N-phenylbenzenesulfonamido) - 93904-37-1P, Acetamide, 2-(p-bromo-N-phenylbenzenesulfonamido)-N,N-diethyl- 93995-09-6P, Acetamide, 2-(p-chloro-N-phenylbenzenesulfonamido)-N,N-diethyl- 93996-27-1P, Acetamide, N,N-diethyl-2-(p-nitro-N-phenylbenzenesulfonamido) - 94263-24-8P, Acetamide, N,N-diethyl-2-(N-phenylbenzenesulfonamido) - 94437-71-5P, Acetamide, N,N-diethyl-2-(N-phenyl-p-toluenesulfonamido) - 95167-60-5P, Acetamide, N,N-diethyl-2-(m-nitro-N-phenylbenzenesulfonamido) - 98981-10-3P, Acetamide, 2-(p-chloro-N-m-tolylbenzenesulfonamido)-N,N-diethyl-
RL: PREP (Preparation)
(preparation of)
RN 88784-29-6 CAPLUS
CN Acetamide, N,N-diethyl-2-(p-iodo-N-phenylbenzenesulfonamido) - (7CI) (CA INDEX NAME)



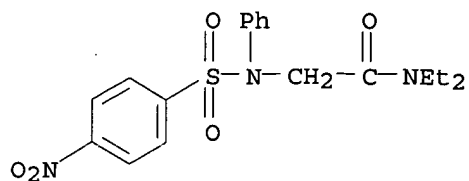
RN 93904-37-1 CAPLUS
CN Acetamide, 2-(p-bromo-N-phenylbenzenesulfonamido)-N,N-diethyl- (7CI) (CA INDEX NAME)



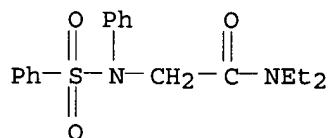
RN 93995-09-6 CAPLUS
CN Acetamide, 2-(p-chloro-N-phenylbenzenesulfonamido)-N,N-diethyl- (7CI) (CA INDEX NAME)



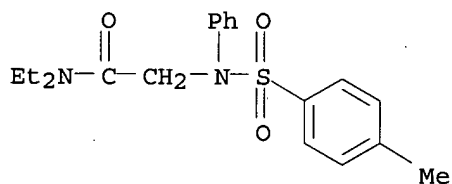
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CN Acetamide, N,N-diethyl-2-(p-nitro-N-phenylbenzenesulfonamido) - (7CI) (CA INDEX NAME)



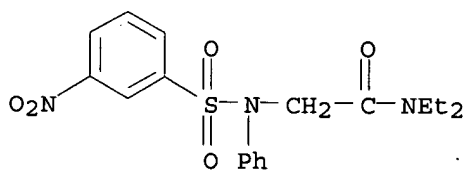
RN 94263-24-8 CAPLUS
 CN Acetamide, N,N-diethyl-2-(N-phenylbenzenesulfonamido) - (7CI) (CA INDEX NAME)



RN 94437-71-5 CAPLUS
 CN Acetamide, N,N-diethyl-2-(N-phenyl-p-toluenesulfonamido) - (7CI) (CA INDEX NAME)



RN 95167-60-5 CAPLUS
 CN Acetamide, N,N-diethyl-2-(m-nitro-N-phenylbenzenesulfonamido) - (7CI) (CA INDEX NAME)



RN 98981-10-3 CAPLUS
 CN Acetamide, 2-(p-chloro-N-m-tolylbenzenesulfonamido)-N,N-diethyl- (7CI) (CA INDEX NAME)

